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FPU Lattices in Multidimensions

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FPU LATTICES IN MULTIDIMENSIONS

by

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Abstract

In a 1955 paper, Enrico Fermi, John Pasta, and Stanislaw Ulam studied a one dimensional, nonlinear dynamical system on an early electronic computer. They were surprised to see the system's original energy configuration recur. The experiment, which has since become known as the "FPU Problem", initiated the field of experimental mathematics, is at the origin of the soliton concept and chaos theory, has sparked revolutions in modern science, and called into question the equipartition hypothesis.

The FPU experiment still has many open questions, not the least of which is an explanation for the recurrence.

In this work, we compare the FPU chain to similar two-dimensional FPU lattices. We did not find original energy configuration recurrence in any of the two dimensional systems we studied, but we note that the systems also did not reach equipartition. Our observations were limited due to accuracy issues with the integrator for some of our systems. We also observed that large, 1024 mass one-dimensional FPU systems acted nearly identical to linear systems.

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1 Background

In a 1955 paper [4], Enrico Fermi, John Pasta, and Stanislaw Ulam studied a one dimensional, nonlinear dynamical system on a "fast" [4, p. 2] electronic computer called MANIAC I[1]. They were surprised to see the system's original energy configuration recur [2–4, 6]. The experiment, which has since become known as the "FPU Problem",[2] initiated the field of experimental mathematics, is at the origin of the soliton concept and chaos theory, and has sparked revolutions in modern science [2, 6]. Physicists require the energy to be equally shared among the modes at the atomic level to get thermodynamics from statistical mechanics (see [6]), but they have been happy to find that large systems thermalize without a complete understanding of why it happens at the microscopic level [3].

The original FPU system is a one dimensional spring and mass system which allowed motion only along the axis (see figure 1). It had no friction and the springs' restoring forces were nonlinear.

Linear springs can be combined with predictable results. The force of two linear springs working together is the sum of their individual forces. Nonlinear springs do not follow this principle (called the Superposition, or Linearity, Principle) [6].

Linear springs' frequency is dependent only on the spring constant and the mass of the oscillating object. Had FPU's lattice been composed of linear springs, the frequency of any object would never change (the mass is constant and the spring constant is, well, constant). So each mode would have retained all of the energy it had at the start and the system would have retained its shape, no matter how long the simulation ran [6].

However, nonlinear springs' frequency is affected by the spring constant, mass, and the amplitude of the oscillations. In other words each oscillating mass affects the amplitude of neighboring masses (because they don't obey the linearity principle) which in turn changes their frequency, which means the energy is shared with other modes [6].

[1] Named *Mathematical Analyzer, Numerical Integrator, and Computer*, in an unsuccessful attempt to discourage using acronyms to name computers [2].

[2] Sometimes FPUT, to reflect the contribution of programmer Mary Tsingou [1].

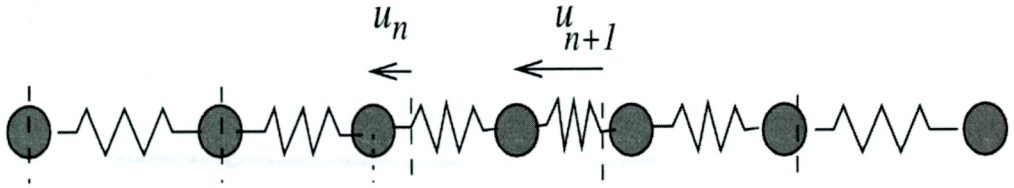


Figure 1: Diagram of the FPU model [lifted from [3]]. Masses move left and right along the axis of the chain, where u_n is mass n's offset from equilibrium. The masses are connected by nonlinear springs.

As a result, FPU expected their system to reach equipartition, where the energy is equally distributed among all of the modes — a state similar to thermal equilibrium in a gas. They started the systems with all of the energy in the first Fourier mode and initially observed the energy being shared among the modes, as expected. But then they noticed nearly all of the energy – 97% of it – return to the first [2, 6]. That is, the original energy configuration reoccurred.

In order to get to thermodynamics from statistical mechanics, physicists require that a gas reach equipartition (see [6]), known to them as the *equipartition hypothesis*. They had thought that nonlinear springs would have been enough to ensure equipartition. But FPU's experiment demonstrated that nonlinearity is not sufficient to guarantee equipartition [6]. So the discovery that a nonlinear system does not automatically thermalize could have thrown a monkey wrench into all of thermodynamics.

The FPU study did more than just introduce a new paradox to the scientific community. It also introduced us to *experimental mathematics*, "computer-based investigations designed to give insight into complex mathematical and physical problems that are inaccessible, at least initially, using more traditional forms of analysis" [6]. From Porter, Zabusky, et al:

> This had far reaching consequences, leading to a complete revolution in the investigation of physical phenomena. The computer is no more used only to perform a calculation that cannot be done by pencil-and-napkin, but to check

> a theoretical conjecture that cannot be proven analytically, or even to provide the theorist with "experimental" results that wait for a mathematical proof: a source of problems, like in a "true laboratory experiment".... Today numerical simulations of condensed matter systems, one reaches such a level of confidence that sometimes it has happened that a laboratory experiment has been questioned because a numerical experiment had given contrary indications. Today, computational physics is an established discipline and it is considered as sort of separated from both theoretical and experimental physics. Students are currently trained in computational physics as in other disciplines, and specialized journals publish the results of the research in this field. This big epistemological and sociological change began with the FPU experiment [2, p. 4].

1.1 Partial Resolution

In 1967, Norman J. Zabusky and Gary Deem found that FPU systems would reach equipartition if only they had enough initial energy. FPU had simply started their system with too little energy to reach equipartition [6].

Later research by E.G.D. Cohen has shown that the FPU recurrences only occur if the total energy per oscillator, (known as the *specific energy*), in the system is below a certain threshold. Above the threshold, the system enters equipartition. Cohen also found that increasing the number of masses reduces the per oscillator threshold. In other words, as the system size increases, it's easier for the system to thermalize. In a system with infintely many masses, the system thermalizes for any level of energy [6, p. 220]. This conforms with what we observe in everyday life.

In 1972, James Tuck and Mary Tsingou-Menzel[3] conducted extensive numerical simulations and put to rest any concern that FPU's recurrences were a result of not running the simulation long enough. They also found that the system experiences even stronger

[3]The original FPU programmer, using her married name.

recurrences, where the first mode recovered even more than 97% of it's initial energy, over even longer time periods, called "superrecurrences" [6, p. 216].

Once it was determined that the system acts as expected for real-world situations, the scientific community seems to have breathed a sigh of relief and forgotten about the issue entirely — there is no mention of it in published work [3].

But we still don't know why the recurrences occur in the first place. This work shows that they do not occur in two dimensions.

2 FPU-Type Lattices

For this work, we are concerned with FPU's β (or cubic) model. The Hamiltonian for such an N mass system is

$$\begin{aligned} H &= T(\dot{\mathbf{u}}) + U(\mathbf{u}) \\ &= \frac{1}{2}\sum_{n=1}^{N} \dot{u}_n^2 + \frac{1}{2}\sum_{n=0}^{N} (u_n - u_{n+1})^2 + \frac{\beta}{4}\sum_{n=0}^{N} (u_n - u_{n+1})^4, \end{aligned} \tag{1}$$

where the spring coefficient and each mass is set to one. Fixed boundaries are represented by $u_0 = u_N = 0$. The equation of motion for mass n is

$$\ddot{u}_n = (u_{n-1} - 2u_n + u_{n+1}) + \beta\left[(u_{n-1} - u_n)^3 - (u_n - u_{n+1})^3\right]. \tag{2}$$

FPU started their systems at rest, with all of the energy in the first linear mode, or

$$u_n(0) = \sin\frac{\pi n}{N} \qquad \text{and} \qquad \dot{u}_n = 0. \tag{3}$$

The Hamiltonian is derived from Newton's Second Law of motion and Hooke's Law.

2.1 Deriving the Linear System

The masses are all unit masses and can only move left and right, along the axis. Each mass' offset is measured as u_n, with their equilibrium point, where it is at rest and has zero net force acting on it, is $u_n = 0$, for all n. The original FPU system had fixed boundaries, which are modeled by letting $u_0 = u_{N+1} = 0$.

From the description, Hooke's Law, and Newton's Second Law of Motion, we can easily derive the system of differential equations which describe the motion of a system with linear springs.

2.1.1 Start with Hooke's Law

Hooke's Law says that the restoring force of a spring is proportional to its extension, or

$$f = -kx,. \tag{4}$$

where f is the spring's restoring force, x is the spring's extension, and k is the spring constant. This paper uses $k = 1$.

Each spring in the FPU lattice is attached to two masses, and so it's extension is measured as the difference in offset of the two masses, or $x_n = u_{n+1} - u_n$. So the force exerted by spring n is

$$S_n = -kx_n = u_n - u_{n+1}. \tag{5}$$

An individual mass of the FPU lattice has two springs acting on it, one on either side. The net force acting on mass n is the sum of the forces from both the spring to its left the one to its right. In other words, the net force acting on m_n is

$$F_n = S_{n-1} - S_n$$

$$= (u_{n-1} - u_n) - (u_n - u_{n+1})$$
$$= u_{n-1} - 2u_n + u_{n+1}. \tag{6}$$

2.1.2 Apply Newton's Second Law

Next, we use Newton's Second Law of Motion, $F = ma$ (the force on an object is equal to its mass times acceleration), and note that the acceleration of m_n is equal to the second derivative of its position with respect to time, represented as $\ddot{u}_n$. In other words, we have that the force on mass n is.

$$F_n = m_n a_n = \ddot{u}_n$$

Plug that into the left of equation (6) and we get

$$\ddot{u}_n = u_{n-1} - 2u_n + u_{n+1} = (u_{n+1} - u_n) - (u_n - u_{n-1}). \tag{7}$$

Equation (7) is the equation of motion for mass n in a one dimensional, linear lattice. It is the controlling equation for this project in that it is the basis of the equations which we will eventually program.

2.1.3 Finding the Hamiltonian

The Hamitonian of a system is defined as

$$H(\mathbf{p}, \mathbf{u}) = T(\mathbf{p}) + U(\mathbf{u}),$$

where T is the kinetic energy, U is the potential energy, $\mathbf{p}$ is a vector of the momentum the masses, $\mathbf{u}$ is a vector of the position of the masses, and

$$\dot{u}_k = \frac{\partial H}{\partial p_k}, \quad \text{and} \quad \dot{p}_k = -\frac{\partial H}{\partial u_k}$$

for all k.

Kinetic energy, by definition, is $T = \frac{1}{2}mv^2$, and momentum is defined to be, $p = mv$. Since all the masses are 1 unit, when we sum over all the masses and we get

$$T(\mathbf{p}) = \frac{1}{2}\sum_{n=1}^{N} mv^2 = \frac{1}{2}\sum_{n=1}^{N} \dot{u}_n^2. \tag{8}$$

Potential energy is stored in the springs between the masses. It is the negative integral of the force the spring exerts times the velocity of the spring with respect to time. The force is the right hand side of (5), $u_n - u_{n+1}$. The springs' change in compression can be calculated as the difference in the speed of the masses on its ends, or the derivative of (5) with respect to time, $\dot{u}_{n+1} - \dot{u}_n$. So the potential energy in spring n is

$$U_n = -\int \mathbf{F}\mathbf{v}\,\mathrm{d}t = -\int (u_n - u_{n+1})(\dot{u}_{n+1} - \dot{u}_n)\,\mathrm{d}t = \frac{1}{2}(u_n - u_{n+1})^2.$$

Details of the third equal by the product rule:

$$\begin{aligned}
&-\int (u_n - u_{n+1})(\dot{u}_{n+1} - \dot{u}_n)\,\mathrm{d}t \\
&\quad = \int u_n \dot{u}_n\,\mathrm{d}t - \int (u_n \dot{u}_{n+1} + u_{n+1}\dot{u}_n)\,\mathrm{d}t + \int u_{n+1}\dot{u}_{n+1}\,\mathrm{d}t \\
&\quad = \int u_n \tfrac{\mathrm{d}u_n}{\mathrm{d}t}\,\mathrm{d}t - \int \left(u_n \tfrac{\mathrm{d}u_{n+1}}{\mathrm{d}t} + u_{n+1}\tfrac{\mathrm{d}u_n}{\mathrm{d}t}\right)\mathrm{d}t + \int u_{n+1}\tfrac{\mathrm{d}u_{n+1}}{\mathrm{d}t}\,\mathrm{d}t \\
&\quad = \int u_n \tfrac{\mathrm{d}u_n}{\mathrm{d}t}\,\mathrm{d}t - \int \tfrac{\mathrm{d}}{\mathrm{d}t}(u_n u_{n+1})\,\mathrm{d}t + \int u_{n+1}\tfrac{\mathrm{d}u_{n+1}}{\mathrm{d}t}\,\mathrm{d}t \\
&\quad = \int u_n\,\mathrm{d}u_n - \int \tfrac{\mathrm{d}}{\mathrm{d}t}(u_n u_{n+1})\,\mathrm{d}t + \int u_{n+1}\,\mathrm{d}u_{n+1} \\
&\quad = \frac{1}{2}u_n^2 - u_n u_{n+1} + \frac{1}{2}u_{n+1}^2 \\
&\quad = \frac{1}{2}(u_n - u_{n+1})^2.
\end{aligned}$$

Sum over all the springs to get the system's potential energy

$$U(\mathbf{u}) = \sum_{n=0}^{N} U_n = \frac{1}{2}\sum_{n=0}^{N}(u_n - u_{n+1})^2, \qquad (u_0 = u_{N+1} = 0). \tag{9}$$

So the Hamiltonian is

$$H(\mathbf{p},\mathbf{u}) = \frac{1}{2}\sum_{n=1}^{N}\dot{u}_n^2 + \frac{1}{2}\sum_{n=0}^{N}(u_n - u_{n+1})^2, \tag{10}$$

with $u_0 = u_{N+1} = 0$.

First, we find

$$\begin{aligned}\dot{u}_k &= \frac{\partial}{\partial p_k}H(\mathbf{p},\mathbf{u}) = \frac{\partial}{\partial p_k}T(\mathbf{p}) + \cancelto{0}{\frac{\partial}{\partial p_k}U(\mathbf{u})} \\ &= \frac{\partial}{\partial p_k}\left(\frac{1}{2}\sum_{n=1}^{N}\frac{p_n^2}{m_n}\right) = \frac{\partial}{\partial p_k}\left(\frac{1}{2}\frac{p_k^2}{m_k}\right) = \frac{p_k}{m_k},\end{aligned}$$

because potential energy is constant with respect to momentum and the derivative with respect to momentum of mass k is zero for all masses $n \neq k$.

Now we find

$$\begin{aligned}\dot{p}_k &= -\frac{\partial}{\partial u_k}H(\mathbf{p},\mathbf{u}) = -\cancelto{0}{\frac{\partial}{\partial u_k}T(\mathbf{p})} - \frac{\partial}{\partial u_k}U(\mathbf{u}) \\ &= \frac{\partial}{\partial u_k}\left[-\frac{1}{2}\sum_{n=0}^{N}(u_n - u_{n+1})^2\right] \\ &= \frac{\partial}{\partial u_k}\left[-\frac{1}{2}(u_{k-1} - u_k)^2 - \frac{1}{2}(u_k - u_{k+1})^2\right] \\ &= (u_{k-1} - u_k) - (u_k - u_{k+1}) \\ &= u_{k-1} - 2u_k - u_{k+1},\end{aligned}$$

because kinetic energy is constant with respect to the position of mass k and the derivative with respect to position of mass k is zero for all masses $n \neq k$.

So we have that $\dot{u}_k = \dfrac{p_k}{m_k}$ and $\dot{p}_k = u_{k-1} - 2u_k - u_{k+1}$. Solve the former for p_k, take the

time derivative and equate to the right side of the latter

$$m_k \ddot{u}_k = \dot{p}_k = u_{k-1} - 2u_k - u_{k+1}.$$

Recall that all masses are 1 mass unit, and arrive at the equation of motion

$$\ddot{u}_k = u_{k-1} - 2u_k - u_{k+1}.$$

2.1.4 Generalize the System

More generally, for an N-mass system we can write

$$\begin{aligned}
\ddot{u}_1 &= u_0 - 2u_1 + u_2 \\
\ddot{u}_2 &= u_1 - 2u_2 + u_3 \\
&\vdots \\
\ddot{u}_N &= u_{N-1} - 2u_N + u_{N+1}.
\end{aligned}$$

Then let

$$\ddot{\mathbf{u}} = \begin{bmatrix} \ddot{u}_1 \\ \ddot{u}_2 \\ \vdots \\ \ddot{u}_N \end{bmatrix}, \qquad \mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{bmatrix}, \qquad \text{and}$$

$$K = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ \vdots & & & \ddots & & & \vdots \\ \vdots & & & & & & \vdots \\ 0 & \dots & & & -1 & 2 & -1 \\ 0 & \dots & & & 0 & -1 & 2 \end{bmatrix},$$

and we can write any N-mass system using

$$\ddot{\mathbf{u}} = -K\mathbf{u}. \tag{11}$$

2.1.5 Reduce the system's Order

The system is a 2^{nd} order differential system. To program it, we reduce it to a first order system.

We introduce a new variable, v such that $v_n = \dot{u}_n$. Then $\dot{v}_n = \ddot{u}_n$, and we can write (7) as the following first order differential system with no derivatives on the right hand sides,

$$\begin{aligned} \dot{u}_n &= v_n \\ \dot{v}_n &= u_{n-1} - 2u_n + u_{n+1}. \end{aligned} \tag{12}$$

For a system of N masses, we write the first order system as

$$\begin{aligned} \dot{u}_1 &= v_1 \\ \dot{u}_2 &= v_2 \\ &\vdots \\ \dot{u}_N &= v_N \end{aligned}$$

$$
\begin{aligned}
\dot{v}_1 &= u_0 - 2u_1 + u_2 \\
\dot{v}_2 &= u_1 - 2u_2 + u_3 \\
&\vdots \\
\dot{v}_N &= u_{N-1} - 2u_N + u_{N+1}.
\end{aligned} \tag{13}
$$

The left side of system (13) is a vector, call it $\dot{\mathbf{u}}$,

$$
\dot{\mathbf{u}} = \begin{bmatrix} \dot{u}_1 \\ \dot{u}_2 \\ \vdots \\ \dot{u}_N \\ \dot{v}_1 \\ \dot{v}_2 \\ \vdots \\ \dot{v}_N \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \\ u_0 - 2u_1 + u_2 \\ u_1 - 2u_2 + u_3 \\ \vdots \\ u_{N-1} - 2u_N + u_{N+1} \end{bmatrix}. \tag{14}
$$

The linear system would be implemented by programming the right side of (14) as a function to be solved by an ODE solver. But we implement the cubic, or β model (which we'll see in (28)).

2.2 Solving the Linear System

Solve the Equation The solution to

$$
\ddot{u} = -ku \tag{15}
$$

is

$$
u(t) = Ce^{i\sqrt{k}t} + C^{\dagger}e^{-i\sqrt{k}t}, \tag{16}
$$

where C and $C^\dagger$ are complex conjugates (so that the solution describes real-valued motion in one dimension).

We expand $C = A + iB$ and $C^\dagger = A - iB$, and simplify

$$\begin{aligned} u(t) &= Ce^{i\sqrt{k}t} + C^\dagger e^{-i\sqrt{k}t} \\ &= \Big(A + iB\Big)\Big(\cos(\sqrt{k}t) + i\sin(\sqrt{k}t)\Big) \\ &\quad + \Big(A - iB\Big)\Big(\cos(\sqrt{k}t) - i\sin(\sqrt{k}t)\Big) \\ &= 2\Big(A\cos(\sqrt{k}t) - B\sin(\sqrt{k}t)\Big) \end{aligned}$$

which describes real valued, oscillating motion. Note that $A = \dfrac{C + C^\dagger}{2}$ and $B = \dfrac{C - C^\dagger}{2i}$ are the Fourier coefficients.

2.2.1 Solve the System

To solve system (11), $\ddot{\mathbf{u}} = -K\mathbf{u}$, of linear springs, let one solution, $\mathbf{u}_1$, be

$$\mathbf{u}_1 = a(t)\mathbf{v}_1, \tag{17}$$

where $a(t)$ is a scalar multiple that varies over time, and $\mathbf{v}_1$ is an eigenvector of K such that $K\mathbf{v}_1 = \lambda_1\mathbf{v}_1$.

We take the second derivative of (17) and equate that to the right hand side of system (11)

$$\ddot{\mathbf{u}}_1 = \ddot{a}\mathbf{v}_1 = -K\mathbf{u}_1 = -K(a\mathbf{v}_1) = -a(K\mathbf{v}_1) = -a\lambda_1\mathbf{v}_1$$

The second and last terms, taken together, imply (since an eigenvector can never be zero)

$$\ddot{a} = -a\lambda_1,$$

which is identical to (15) whose solution, (16), is

$$a(t) = C_1 e^{i\sqrt{\lambda_1}t} + C_1^\dagger e^{-i\sqrt{\lambda_1}t} = 2\left(A_1 \cos(\sqrt{k_1}t) - B_1 \sin(\sqrt{k_1}t)\right).$$

Let $k_n = \sqrt{\lambda_n}$, substitute for $a(t)$ in equation (17), and we find the first solution, an "eigen-solution", to the system is

$$\begin{aligned}\mathbf{u}_1(t) &= \left(C_1 e^{ik_1 t} + C_1^\dagger e^{-ik_1 t}\right)\mathbf{v}_1 \\ &= 2\left(A_1 \cos(k_1 t) - B_1 \sin(k_1 t)\right)\mathbf{v}_1,\end{aligned}$$

assuming that $\lambda_1 > 0$.

In an N-mass system, K is NxN and it has up to N eigenvalues, λ_n $(n = 1..N)$, with corresponding eigenvectors, $\mathbf{v}_n$, and corresponding eigensolutions. Linear combinations of solutions are also solutions (by Linearity Principle). And so the most general solution to $\ddot{\mathbf{u}} = -K\mathbf{u}$, is a combination of the solutions obtained for each eigenvector. Thus, the general solution to the linear system, $\ddot{\mathbf{u}} = -K\mathbf{u}$, is

$$\mathbf{u}(t) = \sum_{j=1}^{N} \mathbf{u}_j(t) = \sum_{j=1}^{N} \left(C_j e^{ik_j t} + C_j^\dagger e^{-ik_j t}\right)\mathbf{v}_j.$$

Since we know the final solution is real numbers, we require C_j and $C_j^\dagger$ to be complex conjugates, $C_j = A_j + iB_j$ and $C_j^\dagger = A_j - iB_j$, and

$$\mathbf{u}(t) = 2\sum_{j=1}^{N} \left(A_j \cos(k_j t) - B_j \sin(k_j t)\right)\mathbf{v}_j. \tag{18}$$

Note that we could apply a few trig identities and represent (18) as

$$\mathbf{u}(t) = \sum_{j=1}^{N} A_j \cos\left(\Omega_j t + \Phi_j\right)\mathbf{v}_j.$$

Notice that A_j, Ω_j, and Φ_j, the amplitude, frequency and phase shift, are all independent of time. That is, in the linear system, if the energy starts in mode 1, then it stays in mode 1.

But we still need the eigenvectors and eigenvalues.

2.2.2 Find the Fourier Coefficients

The initial conditions of the FPU system start the masses stationary and their positions in the first (or low) mode — that is, their offsets are steps of the sine function half way around the unit circle — at $t = 0$

$$u_n(0) = \sin\frac{\pi n}{N} \qquad \text{and} \qquad \dot{u}_n = 0.$$

We use these as

$$\mathbf{u}(0) = \begin{bmatrix} u_1(0) \\ u_2(0) \\ \vdots \\ u_N(0) \end{bmatrix} \qquad \text{and} \qquad \dot{\mathbf{u}}(0) = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

in (18), and it reduces to

$$\mathbf{u}(0) = 2\sum_{n=1}^{N} A_n \mathbf{v}_n = 2\begin{pmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_N \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ A_N \end{pmatrix} = \begin{bmatrix} u_1(0) \\ u_2(0) \\ \vdots \\ u_N(0) \end{bmatrix}.$$

Let $V = \begin{pmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_N \end{pmatrix}$, and we have

$$\mathbf{A} = \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ A_N \end{pmatrix} = \frac{1}{2} V^{-1} \begin{bmatrix} u_1(0) \\ u_2(0) \\ \vdots \\ u_N(0) \end{bmatrix} = \frac{1}{2} V^{\dagger} \begin{bmatrix} u_1(0) \\ u_2(0) \\ \vdots \\ u_N(0) \end{bmatrix} \tag{19}$$

because V is unitary, so it's inverse equals it's conjugate transpose.

Note also that since V is unitary, the dot product of two different columns equals zero, and the dot product of a column with itself equals 1. Since V's columns are eigenvectors of K, and the initial condition, $u_n(0)$ equals the first eigenvector of K, we get that $A_1 = \frac{1}{2}$ and $A_n = 0$ for all $n \neq 1$.

To find the B_ns, we set the derivative of (18) equal to the second initial condition, $\dot{\mathbf{u}}(0) = \mathbf{0}$

$$\dot{\mathbf{u}}(t) = -2 \sum_{n=1}^{N} \left(A_n k_n \sin(k_n t) + B_n k_n \cos(k_n t) \right) \mathbf{v}_n$$

$$\dot{\mathbf{u}}(0) = -2 \sum_{n=1}^{N} B_n k_n \mathbf{v}_n = -2 \begin{pmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_N \end{pmatrix} \begin{pmatrix} B_1 k_1 \\ B_2 k_1 \\ \vdots \\ B_N k_N \end{pmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Therefore,

$$\mathbf{B} = \begin{pmatrix} B_1 k_1 \\ B_2 k_1 \\ \vdots \\ B_N k_N \end{pmatrix} = -\frac{1}{2} V^{-1} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \mathbf{0}, \tag{20}$$

and $B_n = 0$ for all n. In fact, for any system that starts at rest at $t = 0$, we get that the $B_n = 0$ for all n.

Since our system always starts with zero velocity, we can substitute $B_n = 0$ into (18) and reduce the general solution of the linear equation to

$$\mathbf{u}(t) = 2\sum_{n=1}^{N} A_n \cos(k_n t)\mathbf{v}_n.$$

If we also substitute that $A_1 = \frac{1}{2}$ and $A_n = 0$ for all $n \neq 1$, we can simplify the solution to the linear system which which is started with all of its energy as the potential energy in the first mode even further, to

$$\mathbf{u}(t) = \cos(\sqrt{\lambda_1}t)\mathbf{v}_1. \tag{21}$$

Take the time derivative of both sides to find an equation which gives the velocities of the masses

$$\dot{\mathbf{u}}(t) = -\sqrt{\lambda_1}\sin(\sqrt{\lambda_1}t)\mathbf{v}_1. \tag{22}$$

Equations (21)and (22) are used to test our code and our integrator (see section 6.2). We will use a slightly different form of (19) and (20), but with the integrater's output (instead of the initial conditions) to find the Fourier coefficients, As and Bs, at any point in time during the simulation. We will see that solution in (24).

2.2.3 Eigenvalues and Eigenvectors

The eigenvectors, $\mathbf{v}_j$ for $j = 1 \ldots N$, of K for the fixed boundary system's K are

$$\mathbf{v}_j(n) = \sin\left(\frac{j\pi n}{N+1}\right), \tag{23}$$

for mass $n = \ldots N$. These are equally spaced intervals halfway around the unit circle. The matrix $\mathbf{V} = \begin{pmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \ldots & \mathbf{v}_N \end{pmatrix}$ is symmetric.

We check that (23) solves system (11) by taking its second derivative and setting it equals the right hand side of (11). We begin by converting it to exponential form

$$\mathbf{v}_j(n) = \sin\left(\frac{j\pi n}{N+1}\right) = \frac{\omega^{jn} - \omega^{-jn}}{2\mathrm{i}},$$

where $\omega = \mathrm{e}^{\frac{\pi}{N+1}\mathrm{i}}$. In place of the second derivative, we use (2), which is the differential form of the second derivative. We get

$$\begin{aligned}
\ddot{\mathbf{v}}_j(n) &= \mathbf{v}_j(n-1) - 2\mathbf{v}_j(n) + \mathbf{v}_j(n+1) \\
&= \left(\frac{\omega^{j(n-1)} - \omega^{-j(n-1)}}{2\mathrm{i}} - 2\frac{\omega^{jn} - \omega^{-jn}}{2\mathrm{i}} + \frac{\omega^{j(n+1)} - \omega^{-j(n+1)}}{2\mathrm{i}}\right) \\
&= \left(\omega^{-j} + \omega^{j} - 2\right)\left(\frac{\omega^{jn} - \omega^{-jn}}{2\mathrm{i}}\right) \\
&= -\left(2 - \omega^{j} - \omega^{-j}\right)\mathbf{v}_j(n).
\end{aligned}$$

That is, $\ddot{\mathbf{v}}_j(n) = -\left(2 - \omega^{j} - \omega^{-j}\right)\mathbf{v}_j(n)$. Use in (11) to find the eigenvalues

$$\begin{aligned}
\ddot{\mathbf{u}} &= -K\mathbf{u} \\
\ddot{\mathbf{v}}_j(n) &= -K\mathbf{v}_j(n) = -\left(K\mathbf{v}_j(n)\right) = -\left(\lambda_j \mathbf{v}_j(n)\right) \\
&\Rightarrow \\
\lambda_j &= 2 - \omega^{j} - \omega^{-j} = 2 - 2\cos\left(\frac{j\pi}{N+1}\right).
\end{aligned}$$

2.2.4 Transform Matrix

We create the generalized transform matrix, **F**, by normalizing each eigenvector by its magnitude, or the sum of squares,

$$\begin{aligned}
\sum_{n=1}^{N} \mathbf{v}_j(n)^2 &= \sum_{n=1}^{N} \sin\left(\frac{j\pi n}{N+1}\right)^2 \\
&= \sum_{n=1}^{N} \left(\frac{\omega^{jn} - \omega^{-jn}}{2\mathrm{i}}\right)^2 \\
&= -\frac{1}{4}\left(\sum_{n=1}^{N} \omega^{2jn} - \sum_{n=1}^{N} 2 + \sum_{n=1}^{N} \omega^{-2jn}\right) \\
&= -\frac{1}{4}\left(\frac{\omega^{2j} - \omega^{2j(N+1)}}{1-\omega^{2j}} - 2N + \frac{\omega^{-2j} - \omega^{-2j(N+1)}}{1-\omega^{-2j}}\right) \\
&= -\frac{1}{4}(-2-2N) = \frac{N+1}{2},
\end{aligned}$$

where $\omega = \mathrm{e}^{\frac{\pi}{N+1}\mathrm{i}}$ and using the geometric series rule and noting that $\omega^{N+1} = -1$. Since all the vectors have the same magnitude, we get

$$\mathbf{F} = \frac{\mathbf{V}^{\dagger}}{\sqrt{\frac{N+1}{2}}}. \tag{24}$$

Matrix **F** is the normalized transpose of the matrix of eigenvectors, **V**. We use it in (19) and (20), but with the integrator's output (instead of with the initial conditions) to find the Fourier coefficients, the **A**s and **B**s, of the simulation. That is, at any time t, we can find the Fourier coefficients of the system's condition, $\mathbf{u}(t)$, with

$$\mathbf{w} = \mathbf{F}\mathbf{u}(t)$$

$$\dot{\mathbf{w}} = \mathbf{F}\dot{\mathbf{u}}(t)$$

2.3 Energy in Fourier Space

Hamiltonian as a Matrix We can write the linear potential energy, (9), in matrix form as follows

$$
\begin{aligned}
2u &= \sum_{n=0}^{N} (u_n - u_{n+1})^2 = \sum_{n=0}^{N} \left(u_n^2 - 2u_n u_{n+1} + u_{n+1}^2 \right) \\
&= \left(u_0^2 - 2u_0 u_1 + u_1^2 \right) + \left(u_1^2 - 2u_1 u_2 + u_2^2 \right) + \cdots \\
&\quad + \left(u_{N-1}^2 - 2u_{N-1} u_N + u_N^2 \right) + \left(u_N^2 - 2u_N u_{N+1} + u_{N+1}^2 \right) \\
&= \left(-u_0 u_1 + 2u_1^2 - u_1 u_2 \right) + \left(-u_1 u_2 + 2u_2^2 - u_2 u_3 \right) + \cdots \\
&\quad + \left(-u_{N-2} u_{N-1} + 2u_{N-1}^2 - u_{N-1} u_N \right) + \left(-u_{N-1} u_N + 2u_N^2 - u_N u_{N+1} \right) \\
&= \sum_{n=1}^{N} (-u_{n-1} u_n + 2u_n^2 - u_n u_{n+1}) \\
&= \begin{bmatrix} \cdots, -u_{n-1} + 2u_n - u_n u_{n+1}, \cdots \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{bmatrix} \\
&= \begin{bmatrix} u_1 & u_2 & \cdots & u_N \end{bmatrix} \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ \vdots & & & & & & \vdots \\ \vdots & & & & & & \vdots \\ 0 & \dots & & & -1 & 2 & -1 \\ 0 & \dots & & & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{bmatrix} \\
&= \mathbf{u}^\intercal K \mathbf{u}. \\
U &= \frac{1}{2} \mathbf{u}^\intercal K \mathbf{u}.
\end{aligned}
$$

Note that the third line (or fourth equal sign) above is achieved by dropping the terms u_0^2 and u_{N+1}^2 and one of the two terms for each of $-u_0 u_1$ and $-u_N u_{N+1}$ from the previous line. We can do so because $u_0 = u_{N+1} = 0$.

Kinetic energy, (8), in matrix form is

$$T = \frac{1}{2}\sum_{n=1}^{N} \dot{u}_n^2 = \frac{1}{2}\begin{bmatrix} \dot{u}_1 & \dot{u}_2 & \cdots & \dot{u}_N \end{bmatrix} \begin{bmatrix} \dot{u}_1 \\ \dot{u}_2 \\ \vdots \\ \dot{u}_N \end{bmatrix} = \frac{1}{2}\dot{\mathbf{u}}^\mathsf{T}\dot{\mathbf{u}}.$$

Thus, the Hamiltonian, (1), can be written in matrix form as

$$H = \frac{1}{2}\dot{\mathbf{u}}^\mathsf{T}\dot{\mathbf{u}} + \frac{1}{2}\mathbf{u}^\mathsf{T}K\mathbf{u}$$

2.3.1 Energy in Fourier Space

We calculate the energy in each linear mode using a generalized Fourier transform. We use the transposed, normalized eigenvector matrix, $\mathbf{F}$, defined in (24), as the transform matrix. Start with the equation for (twice the) energy

$$2H = \mathbf{u}^\mathsf{T}K\mathbf{u} + \dot{\mathbf{u}}^\mathsf{T}\dot{\mathbf{u}}.$$

Recall (11), $\ddot{\mathbf{u}} = -K\mathbf{u}$. Let $\mathbf{w} = \mathbf{F}\mathbf{u}$, then $\dot{\mathbf{w}} = \mathbf{F}\dot{\mathbf{u}}$ (because $\mathbf{F}$ is constant). From linear algebra, we have that $\mathbf{DF} = \mathbf{FK}$ (so that $\mathbf{D} = \mathbf{FKF}^{-1}$) and that $\mathbf{F}^{-1} = \mathbf{F}^\dagger = \mathbf{F}^\mathsf{T}$ (because it's unitary and real valued, aka orthogonal). Then we have

$$\begin{aligned}
2H &= \mathbf{u}^\mathsf{T}K\mathbf{u} + \dot{\mathbf{u}}^\mathsf{T}\dot{\mathbf{u}} \\
&= \mathbf{u}^\mathsf{T}(\mathbf{F}^{-1}\mathbf{F})K(\mathbf{F}^{-1}\mathbf{F})\mathbf{u} + \dot{\mathbf{u}}^\mathsf{T}(\mathbf{F}^{-1}\mathbf{F})\dot{\mathbf{u}} \\
&= \mathbf{u}^\mathsf{T}(\mathbf{F}^\mathsf{T}\mathbf{F})K(\mathbf{F}^\mathsf{T}\mathbf{F})\mathbf{u} + \dot{\mathbf{u}}^\mathsf{T}(\mathbf{F}^\mathsf{T}\mathbf{F})\dot{\mathbf{u}} \\
&= (\mathbf{u}^\mathsf{T}\mathbf{F}^\mathsf{T})(\mathbf{F}K\mathbf{F}^\mathsf{T})(\mathbf{F}\mathbf{u}) + (\dot{\mathbf{u}}^\mathsf{T}\mathbf{F}^\mathsf{T})(\mathbf{F}\dot{\mathbf{u}}) \\
&= (\mathbf{F}\mathbf{u})^\mathsf{T}D(\mathbf{F}\mathbf{u}) + (\mathbf{F}\dot{\mathbf{u}})^\mathsf{T}(\mathbf{F}\dot{\mathbf{u}}) \\
&= \mathbf{w}^\mathsf{T}D\mathbf{w} + \dot{\mathbf{w}}^\mathsf{T}\dot{\mathbf{w}}.
\end{aligned}$$

The linear Hamiltonian, in Fourier space, is thus

$$H = \frac{1}{2}\mathbf{w}^{\mathsf{T}} D\mathbf{w} + \frac{1}{2}\dot{\mathbf{w}}^{\mathsf{T}}\dot{\mathbf{w}}. \tag{25}$$

We already know, from section 2.4.1 that H is constant. It should, of course, be the same value in Euclidean space as it is in Fourier space.

Therefore, to find the energy in linear mode j, we first convert the position and velocity data output by the integrator to Fourier space

$$\mathbf{w} = \mathbf{F}\mathbf{u}$$

$$\dot{\mathbf{w}} = \mathbf{F}\dot{\mathbf{u}}.$$

Then calculate the energy in each mode using (25). Each column of H will contain the energy, over time, in one mode.

2.4 The β Model

Deriving the Nonlinear System We add a cubic force to each spring's restoring force, (4), so that it becomes

$$f = -kx - \beta x^3, \tag{26}$$

where β is a constant which regulates the strength of the nonlinear force relative to the linear force.

Then the force exerted by a spring becomes (recall that $k = 1$)

$$S_n = -x_n + \beta x_n^3 = (u_n - u_{n+1}) + \beta (u_n - u_{n+1})^3.$$

The kinetic energy of each mass is unchanged, so the equation for kinetic energy of the sys-

tem remains (8). But the nonlinear term must be added to the potential energy calculation, (9), which becomes

$$U(\mathbf{u}) = \frac{1}{2}\sum_{n=0}^{N}(u_n - u_{n+1})^2 + \frac{\beta}{4}\sum_{n=0}^{N}(u_n - u_{n+1})^4. \tag{27}$$

Then the Hamiltonian becomes

$$\begin{aligned} H(\mathbf{p},\mathbf{u}) &= T(\mathbf{p}) + U(\mathbf{u}) \\ &= \frac{1}{2}\sum_{n=1}^{N}\dot{u}_n^2 \\ &\quad + \frac{1}{2}\sum_{n=0}^{N}(u_n - u_{n+1})^2 + \frac{\beta}{4}\sum_{n=0}^{N}(u_n - u_{n+1})^4, \end{aligned}$$

with $(u_0 = u_{N+1} = 0)$. This matches (1) and is the system that FPU used in their original experiment [4].

Following the same procedure as in 2.1.3, we find the equation of motion, (2), becomes

$$\begin{aligned} \ddot{u}_n = &\left[(u_{n-1} - u_n) - (u_n - u_{n+1})\right] \\ &+ \beta\left[(u_{n-1} - u_n)^3 - (u_n - u_{n+1})^3\right]. \end{aligned} \tag{28}$$

This is the controlling equation of the 1 dimensional FPU model. It is the function we send to the ODE solver, SUNDIALS. After reducing the order by introducing $v_n = \dot{u}_n$, as in section 2.1.5. The result is

$$\begin{aligned} \dot{u}_1 &= v_1 \\ \dot{u}_2 &= v_2 \\ &\vdots \\ \dot{u}_N &= v_N \\ \dot{v}_1 &= \left[(u_0 - 2u_1 + u_2)\right] + \beta\left[(u_0 - u_1)^3 - (u_1 - u_2)^3\right] \end{aligned} \tag{29}$$

$$\dot{v}_2 = \left[(u_1 - 2u_2 + u_3)\right] + \beta\left[(u_1 - u_2)^3 - (u_2 - u_3)^3\right]$$

$$\vdots$$

$$\dot{v}_N = \left[(u_{N-1} - 2u_N + u_{N+1})\right] + \beta\left[(u_{N-1} - u_N)^3 - (u_N - u_{N+1})^3\right].$$

There is no matrix representation of a nonlinear Hamiltonian.

2.4.1 Energy in the β Model

Energy in the β model is conserved. Start with its time derivative

$$\begin{aligned}
\dot{H} &= \sum_{n=0}^{N} (u_n - u_{n+1})(\dot{u}_n - \dot{u}_{n+1}) \\
&\quad + \beta \sum_{n=0}^{N} (u_n - u_{n+1})^3 (\dot{u}_n - \dot{u}_{n+1}) + \sum_{n=1}^{N} \dot{u}_n \ddot{u}_n \\
&= \sum_{n=0}^{N} (u_n - u_{n+1})\dot{u}_n - \sum_{n=0}^{N} (u_n - u_{n+1})\dot{u}_{n+1} \\
&\quad + \beta \sum_{n=0}^{N} (u_n - u_{n+1})^3 \dot{u}_n - \beta \sum_{n=0}^{N} (u_n - u_{n+1})^3 \dot{u}_{n+1} + \sum_{n=1}^{N} \dot{u}_n \ddot{u}_n.
\end{aligned}$$

Since $u_0 = \dot{u}_0 = 0$, we can eliminate the $n = 0$ index from the first and third terms. Then we shift the second and fourth terms' indices and note that $u_{N+1} = \dot{u}_{N+1} = 0$, allowing us to remove the $n = N + 1$ terms.

$$\begin{aligned}
\dot{H} &= \sum_{n=1}^{N} (u_n - u_{n+1})\dot{u}_n - \sum_{n=0}^{N} (u_n - u_{n+1})\dot{u}_{n+1} \\
&\quad + \beta \sum_{n=1}^{N} (u_n - u_{n+1})^3 \dot{u}_n - \beta \sum_{n=0}^{N} (u_n - u_{n+1})^3 \dot{u}_{n+1} + \sum_{n=1}^{N} \dot{u}_n \ddot{u}_n \\
&= \sum_{n=1}^{N} (u_n - u_{n+1})\dot{u}_n - \sum_{n=1}^{N+1} (u_{n-1} - u_n)\dot{u}_n \\
&\quad + \beta \sum_{n=1}^{N} (u_n - u_{n+1})^3 \dot{u}_n - \beta \sum_{n=1}^{N+1} (u_{n-1} - u_n)^3 \dot{u}_n + \sum_{n=1}^{N} \dot{u}_n \ddot{u}_n \\
&= \sum_{n=1}^{N} (u_n - u_{n+1})\dot{u}_n - \sum_{n=1}^{N} (u_{n-1} - u_n)\dot{u}_n
\end{aligned}$$

$$+\beta\sum_{n=1}^{N}(u_n-u_{n+1})^3\dot{u}_n-\beta\sum_{n=1}^{N}(u_{n-1}-u_n)^3\dot{u}_n+\sum_{n=1}^{N}\dot{u}_n\ddot{u}_n.$$

Finally, since the indices are now aligned, we can factor out $\dot{u}_n$

$$\begin{aligned}\dot{H}=-\sum_{n=1}^{N}\Big[&\big((u_{n-1}-u_n)-(u_n-u_{n+1})\big)\\&+\beta\Big((u_{n-1}-u_n)^3-(u_n-u_{n+1})^3\Big)-\ddot{u}_n\Big]\dot{u}_n.\end{aligned}$$

The expression in brackets is the equation of motion, (28), which equals zero, proving that the energy is constant in this system.

2.4.2 Initial Energy

The system starts at rest, so initially has no kinetic energy. The masses' initial positions at $t=0$, as given by (3) are

$$u_n(0)=\sin\left(\frac{n\pi}{N+1}\right).$$

Substitute the IC, (3), into (9) (which is also the first term of (27)) to find the initial potential energy due to the linear term. We get

$$\begin{aligned}2U&=\sum_{n=0}^{N}(u_n-u_{n+1})^2\\&=\sum_{n=0}^{N}\left(\sin\left(\frac{n\pi}{N+1}\right)-\sin\left(\frac{(n+1)\pi}{N+1}\right)\right)^2\\&=\sum_{n=0}^{N}\left(\frac{e^{i\frac{n\pi}{N+1}}-e^{-i\frac{n\pi}{N+1}}}{2i}-\frac{e^{i\frac{(n+1)\pi}{N+1}}-e^{-i\frac{(n+1)\pi}{N+1}}}{2i}\right)^2\\&=-\frac{1}{4}\sum_{n=0}^{N}\left(\omega^n-\omega^{-n}-\omega^{n+1}+\omega^{-(n+1)}\right)^2,\end{aligned}$$

where $\omega=e^{i\frac{\pi}{N+1}}$. Continuing to calculate the initial energy by squaring, distributing the

summation, and applying the geometric series and summation rules, we get

$$
\begin{aligned}
-8H &= \sum_{n=0}^{N}\left(\omega^{n}-\omega^{-n}-\omega^{n+1}+\omega^{-(n+1)}\right)^{2} \\
&= \sum_{n=0}^{N}\Big(\omega^{2n}-2\omega^{2n+1}+2\omega^{-1}+\omega^{-2n}+2\omega \\
&\qquad\qquad -2\omega^{-2n-1}+\omega^{2n+2}+\omega^{-2n-2}-4\Big) \\
&= \sum_{n=0}^{N}\omega^{2n+2}-2\sum_{n=0}^{N}\omega^{2n+1}+\sum_{n=0}^{N}\omega^{2n}+2\sum_{n=0}^{N}\omega+2\sum_{n=0}^{N}\omega^{-1} \\
&\quad +\sum_{n=0}^{N}\omega^{-2n}-2\sum_{n=0}^{N}\omega^{-2n-1}+\sum_{n=0}^{N}\omega^{-2n-2}-\sum_{n=0}^{N}4 \\
&= \omega^{2}\sum_{n=0}^{N}\omega^{2n}-2\omega\sum_{n=0}^{N}\omega^{2n}+\sum_{n=0}^{N}\omega^{2n}+2\sum_{n=0}^{N}\omega+2\sum_{n=0}^{N}\omega^{-1} \\
&\quad +\sum_{n=0}^{N}\omega^{-2n}-2\omega^{-1}\sum_{n=0}^{N}\omega^{-2n}+\omega^{-2}\sum_{n=0}^{N}\omega^{-2n}-\sum_{n=0}^{N}4 \\
&= \omega^{2}\left(\frac{1-\omega^{2(N+1)}}{1-\omega^{2}}\right)-2\omega\left(\frac{1-\omega^{2(N+1)}}{1-\omega^{2}}\right)+\left(\frac{1-\omega^{2(N+1)}}{1-\omega^{2}}\right) \\
&\quad +2(N+1)\omega+2(N+1)\omega^{-1}+\left(\frac{1-\omega^{-2(N+1)}}{1-\omega^{-2}}\right) \\
&\quad -2\omega\left(\frac{1-\omega^{-2(N+1)}}{1-\omega^{-2}}\right)+\omega^{2}\left(\frac{1-\omega^{-2(N+1)}}{1-\omega^{-2}}\right)-4(N+1).
\end{aligned}
$$

The last step by the geometric series. Note that $\omega^{N+1}=\left(e^{i\frac{\pi}{N+1}}\right)^{N+1}=e^{i\pi}=-1$, therefore $\omega^{2(N+1)}=\omega^{-2(N+1)}=1$, and the 1st, 2nd, 3rd, 6th, 7th and 8th terms above equal zero. (In fact, for all even integers v, $\sum_{n=0}^{N}\omega^{vn}=0$.) So we get

$$
\begin{aligned}
-8H &= 2(N+1)\omega+2(N+1)\omega^{-1}-4(N+1) \\
&= 2N\left(\omega+\omega^{-1}\right)+2\left(\omega+\omega^{-1}\right)-4N-4 \\
&= 4N\cos\left(\frac{\pi}{N+1}\right)+4\cos\left(\frac{\pi}{N+1}\right)-4N-4 \\
&= 4(N+1)\left(\cos\frac{\pi}{N+1}-1\right).
\end{aligned}
$$

And so the initial energy due to the linear terms is

$$H = \frac{1}{2}(N+1)\left(1-\cos\frac{\pi}{N+1}\right). \tag{30}$$

Now we substitute the initial conditions, (3), into the right term of (27). We get

$$\begin{aligned}\frac{\beta}{4}\sum_{n=0}^{N}(u_n-u_{n+1})^4 &= \frac{\beta}{4}\sum_{n=0}^{N}\left(\frac{\omega^n-\omega^{-n}}{2\mathrm{i}}-\frac{\omega^{n+1}-\omega^{-(n+1)}}{2\mathrm{i}}\right)^4\\ &= \frac{\beta}{64}\sum_{n=0}^{N}\left(\omega^n-\omega^{-n}-\omega^{n+1}-\omega^{-(n+1)}\right)^4,\end{aligned}$$

where $\omega = \mathrm{e}^{\mathrm{i}\frac{\pi}{N+1}}$.

We use the rule that $\sum_{n=0}^{N}\omega^{vn}=0$ for all even integers v again and expand the above and continue with only the terms which have odd exponents

$$\begin{aligned}&\sum_{n=0}^{N}\left(\omega^n-\omega^{-n}-\omega^{n+1}-\omega^{-(n+1)}\right)^4\\ &\quad=\sum_{n=0}^{N}\left(36-24\omega-24\omega^{-1}+6\omega^2+6\omega^{-2}\right)\\ &\quad=\sum_{n=0}^{N}\left(36-48\cos\left(\frac{\pi}{N+1}\right)+12\cos\left(\frac{2\pi}{N+1}\right)\right)\\ &\quad=(N+1)\left(36-48\cos\left(\frac{\pi}{N+1}\right)+12\cos\left(\frac{2\pi}{N+1}\right)\right)\\ &\quad=12(N+1)\left(3-4\cos\left(\frac{\pi}{N+1}\right)+\cos\left(\frac{2\pi}{N+1}\right)\right).\end{aligned}$$

Finally, multiply by the factor $\frac{\beta}{64}$ (that we didn't retype in the last step) and add to (30) to get the energy in the nonlinear system

$$\begin{aligned}H = &\frac{1}{2}(N+1)\left(3-4\cos\left(\frac{\pi}{N+1}\right)+\cos\left(\frac{2\pi}{N+1}\right)\right)\\ &+\frac{3\beta}{16}(N+1)\left(3-4\cos\left(\frac{\pi}{N+1}\right)+\cos\left(\frac{2\pi}{N+1}\right)\right).\end{aligned} \tag{31}$$

We use this equation to confirm the energy levels in our code (see section 6.2).

This has been confirmed numerically. Note that energy is a function of system size, N, initial condition's amplitude, A and β.

2.5 Vertical Motion

The system is one dimensional and the masses move horizontally along the axis line. But we can just as easily imagine the masses moving vertically (perpendicular to the axis), with horizontal bars that hold them in place. The bar of each mass is connected to the horizontal bar of the next mass by a vertical spring. In this case, our system is still accurately modeled by the system described by the Hamiltonian (1). We can now proceed to the two dimension model picturing the masses as moving up and down.

3 Two Dimensional FPU Lattices

3.1 Deriving the 2D System

In two dimensions, we have a square $N \times N$ matrix and we notate each masses' position with a double subscript. The system is akin to having two one dimensional systems at right angles to each other. So the equation for potential energy is

$$\begin{aligned} U(\mathbf{u}) = &\frac{1}{2}\sum_{m=0}^{N}\sum_{n=0}^{N}\left[\left(u_{m,n}-u_{m+1,n}\right)^2+\left(u_{m,n}-u_{m,n+1}\right)^2\right] \\ &+\frac{\beta}{4}\sum_{m=0}^{N}\sum_{n=0}^{N}\left[\left(u_{m,n}-u_{m+1,n}\right)^4+\left(u_{m,n}-u_{m,n+1}\right)^4\right]. \end{aligned} \tag{32}$$

The resulting Hamiltonian for the 2-dimension β model is

$$\begin{aligned} H(\mathbf{p},\mathbf{u}) &= T(\mathbf{p})+U(\mathbf{u}) \\ &= \frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}\dot{u}_{m,n}^2 \end{aligned}$$

$$+\frac{1}{2}\sum_{m=0}^{N}\sum_{n=0}^{N}\left[\left(u_{m,n}-u_{m+1,n}\right)^2+\left(u_{m,n}-u_{m,n+1}\right)^2\right]$$
$$+\frac{\beta}{4}\sum_{m=0}^{N}\sum_{n=0}^{N}\left[\left(u_{m,n}-u_{m+1,n}\right)^4+\left(u_{m,n}-u_{m,n+1}\right)^4\right], \tag{33}$$

where $u_{m,n}$ is the offset from equilibrium ($u_{m,n}=0$) of mass $m_{m,n}$, and $m,n=1,2..N$. Fixed boundaries are modeled as $u_{0,n}=u_{N+1,n}=u_{m,0}=u_{m,N+1}=0$. Applying the definition of Hamiltonian from 2.1.3, yields

$$\begin{aligned}\ddot{u}_{m,n} &= (u_{m-1,n}-u_{m,n})+(u_{m+1,n}-u_{m,n}) \\ &\quad +(u_{m,n-1}-u_{m,n})+(u_{m,n+1}-u_{m,n}) \\ &\quad +\beta\left[(u_{m-1,n}-u_{m,n})^3+(u_{m+1,n}-u_{m,n})^3\right. \\ &\quad \left.+(u_{m,n-1}-u_{m,n})^3+(u_{m,n+1}-u_{m,n})^3\right].\end{aligned} \tag{34}$$

The masses are all started at rest, with all of the energy in the first mode. That is, the initial condition is

$$u_{m,n}(0)=\sin\left(\frac{m\pi}{N+1}\right)\sin\left(\frac{n\pi}{N+1}\right) \qquad \text{and} \qquad \dot{u}_{m,n}(0)=0. \tag{35}$$

3.1.1 Generalize the 2D Linear System

Next, we let

$$\ddot{\mathbf{u}} = \begin{bmatrix} \ddot{u}_{1,1} \\ \ddot{u}_{1,2} \\ \vdots \\ \ddot{u}_{1,N} \\ \ddot{u}_{2,1} \\ \vdots \\ \ddot{u}_{2,N} \\ \vdots \\ \ddot{u}_{N,N} \end{bmatrix}, \quad \text{and} \quad \mathbf{u} = \begin{bmatrix} u_{1,1} \\ u_{1,2} \\ \vdots \\ u_{1,N} \\ u_{2,1} \\ \vdots \\ u_{2,N} \\ \vdots \\ u_{N,N} \end{bmatrix},$$

and let the coefficient matrix, K, be

$$K = \begin{pmatrix} \mathbf{C} & \mathbf{I} & \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{I} & \mathbf{C} & \mathbf{I} & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{O} & \mathbf{I} & \mathbf{C} & \mathbf{I} & \cdots & \mathbf{O} \\ \vdots & & & \ddots & & \vdots \\ \mathbf{O} & \cdots & & \mathbf{I} & \mathbf{C} & \mathbf{I} \\ \mathbf{O} & \cdots & & \mathbf{O} & \mathbf{I} & \mathbf{C} \end{pmatrix},$$

where $\mathbf{C}$ is NxN

$$\mathbf{C} = \begin{pmatrix} 4 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 4 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 4 & -1 & \cdots & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & \cdots & & -1 & 4 & -1 \\ 0 & \cdots & & 0 & -1 & 4 \end{pmatrix},$$

and $\mathbf{I}$ is the $N \times N$ identity, and $\mathbf{O}$ is $N \times N$ of zeros. Then we can write the linear system as

$$\ddot{\mathbf{u}} = -K\mathbf{u},$$

(which is exactly like (11)).

For example, in a 4×4 linear system, we have

$$\ddot{u}_{1,1} = u_{0,1} + u_{2,1} + u_{1,0} - 4u_{1,1} + u_{1,2}$$

$$\ddot{u}_{1,2} = u_{0,2} + u_{2,2} + u_{1,1} - 4u_{1,2} + u_{1,3}$$

$$\ddot{u}_{1,3} = u_{0,3} + u_{2,3} + u_{1,2} - 4u_{1,3} + u_{1,4}$$

$$\ddot{u}_{1,4} = u_{0,4} + u_{2,4} + u_{1,3} - 4u_{1,4} + u_{1,5}$$

$$\ddot{u}_{2,1} = u_{1,1} + u_{3,1} + u_{2,0} - 4u_{2,1} + u_{2,2}$$

$$\ddot{u}_{2,2} = u_{1,2} + u_{3,2} + u_{2,1} - 4u_{2,2} + u_{2,3}$$

$$\ddot{u}_{2,3} = u_{1,3} + u_{3,3} + u_{2,2} - 4u_{2,3} + u_{2,4}$$

$$\ddot{u}_{2,4} = u_{1,4} + u_{3,4} + u_{2,3} - 4u_{2,4} + u_{2,5}$$

$$\ddot{u}_{3,1} = u_{2,1} + u_{4,1} + u_{3,0} - 4u_{3,1} + u_{3,2}$$

$$\ddot{u}_{3,2} = u_{2,2} + u_{4,2} + u_{3,1} - 4u_{3,2} + u_{3,3}$$

$$\ddot{u}_{3,3} = u_{2,3} + u_{4,3} + u_{3,2} - 4u_{3,3} + u_{3,4}$$

$$\ddot{u}_{3,4} = u_{2,4} + u_{4,4} + u_{3,3} - 4u_{3,4} + u_{3,5}$$

$$\ddot{u}_{4,1} = u_{3,1} + u_{5,1} + u_{4,0} - 4u_{4,1} + u_{4,2}$$

$$\ddot{u}_{4,2} = u_{3,2} + u_{5,2} + u_{4,1} - 4u_{4,2} + u_{4,3}$$

$$\ddot{u}_{4,3} = u_{3,3} + u_{5,3} + u_{4,2} - 4u_{4,3} + u_{4,4}$$

$$\ddot{u}_{4,4} = u_{3,4} + u_{5,4} + u_{4,3} - 4u_{4,4} + u_{4,5},$$

which simplifies (with fixed boundaries) to

$$\ddot{u}_{1,1} = u_{2,1} \qquad - 4u_{1,1} + u_{1,2}$$

$$\ddot{u}_{1,2} = u_{2,2} + u_{1,1} - 4u_{1,2} + u_{1,3}$$

$$\ddot{u}_{1,3} = u_{2,3} + u_{1,2} - 4u_{1,3} + u_{1,4}$$

$$\ddot{u}_{1,4} = u_{2,4} + u_{1,3} - 4u_{1,4}$$

$$\ddot{u}_{2,1} = u_{1,1} + u_{3,1} \qquad - 4u_{2,1} + u_{2,2}$$

$$\ddot{u}_{2,2} = u_{1,2} + u_{3,2} + u_{2,1} - 4u_{2,2} + u_{2,3}$$

$$\ddot{u}_{2,3} = u_{1,3} + u_{3,3} + u_{2,2} - 4u_{2,3} + u_{2,4}$$

$$\ddot{u}_{2,4} = u_{1,4} + u_{3,4} + u_{2,3} - 4u_{2,4}$$

$$\ddot{u}_{3,1} = u_{2,1} + u_{4,1} \qquad - 4u_{3,1} + u_{3,2}$$

$$\ddot{u}_{3,2} = u_{2,2} + u_{4,2} + u_{3,1} - 4u_{3,2} + u_{3,3}$$

$$\ddot{u}_{3,3} = u_{2,3} + u_{4,3} + u_{3,2} - 4u_{3,3} + u_{3,4}$$

$$\ddot{u}_{3,4} = u_{2,4} + u_{4,4} + u_{3,3} - 4u_{3,4}$$

$$\ddot{u}_{4,1} = u_{3,1} \qquad - 4u_{4,1} + u_{4,2}$$

$$\ddot{u}_{4,2} = u_{3,2} + u_{4,1} - 4u_{4,2} + u_{4,3}$$

$$\ddot{u}_{4,3} = u_{3,3} + u_{4,2} - 4u_{4,3} + u_{4,4}$$

$$\ddot{u}_{4,4} = u_{3,4} + u_{4,3} - 4u_{4,4}.$$

Then K is the following 16×16 matrix (zeros replaced by spaces for readability)

$$K = \begin{pmatrix}
4 & -1 & & & -1 & & & & & & & & & & & \\
-1 & 4 & -1 & & & -1 & & & & & & & & & & \\
 & -1 & 4 & -1 & & & -1 & & & & & & & & & \\
 & & -1 & 4 & & & & -1 & & & & & & & & \\
-1 & & & & 4 & -1 & & & -1 & & & & & & & \\
 & -1 & & & -1 & 4 & -1 & & & -1 & & & & & & \\
 & & -1 & & & -1 & 4 & -1 & & & -1 & & & & & \\
 & & & -1 & & & -1 & 4 & & & & -1 & & & & \\
 & & & & -1 & & & & 4 & -1 & & & -1 & & & \\
 & & & & & -1 & & & -1 & 4 & -1 & & & -1 & & \\
 & & & & & & -1 & & & -1 & 4 & -1 & & & -1 & \\
 & & & & & & & -1 & & & -1 & 4 & & & & -1 \\
 & & & & & & & & -1 & & & & 4 & -1 & & \\
 & & & & & & & & & -1 & & & -1 & 4 & -1 & \\
 & & & & & & & & & & -1 & & & -1 & 4 & -1 \\
 & & & & & & & & & & & -1 & & & -1 & 4
\end{pmatrix}.$$

3.1.2 Reduce the 2D System's Order

For programming, we reduce the system to a first order system by introducing $v_n = \dot{u}_n$, just as in section 2.1.5. Then (34) becomes

$$\dot{u}_{m,n} = v_{m,n}$$

$$\dot{v}_{m,n} = \left[(u_{m-1,n} - u_{m,n}) + (u_{m+1,n} - u_{m,n}) \right.$$

$$\left. + (u_{m,n-1} - u_{m,n}) + (u_{m,n+1} - u_{m,n})\right]$$

$$+ \beta \left[(u_{m-1,n} - u_{m,n})^3 + (u_{m+1,n} - u_{m,n})^3 \right.$$

$$+(u_{m,n-1}-u_{m,n})^3+(u_{m,n+1}-u_{m,n})^3\Big].$$

By letting $v_{j,k}=\dot{u}_{j,k}$, we can write an $N\times N$ system as a first order system

$$\begin{aligned}
\dot{u}_{1,1} &= v_{1,1}\\
&\vdots\\
\dot{u}_{1,N} &= v_{1,N}\\
&\vdots\\
\dot{u}_{N,N} &= v_{N,N}\\
\dot{v}_{1,1} &= \big[(u_{0,1}-u_{1,1})+(u_{2,1}-u_{1,1})\\
&\qquad +(u_{1,0}-u_{1,1})+(u_{1,2}-u_{1,1})\big]\\
&\quad +\beta\Big[(u_{0,1}-u_{1,1})^3+(u_{2,1}-u_{1,1})^3\\
&\qquad +(u_{1,0}-u_{1,1})^3+(u_{1,2}-u_{1,1})^3\Big]\\
&\vdots\\
&\vdots\\
\dot{v}_{N,N} &= \big[(u_{N-1,N}-u_{N,N})+(u_{N+1,N}-u_{N,N})\\
&\qquad +(u_{N,N-1}-u_{N,N})+(u_{N,N+1}-u_{N,N})\big]\\
&\quad +\beta\Big[(u_{N-1,N}-u_{N,N})^3+(u_{N+1,N}-u_{N,N})^3\\
&\qquad +(u_{N,N-1}-u_{N,N})^3+(u_{N,N+1}-u_{N,N})^3\Big].
\end{aligned}\tag{36}$$

The right hand side of system (36) is the 2 dimensional function that what we pass to the ODE solver, analogous to (29).

3.2 Solving the 2-D Linear System

3.2.1 Solving the Continuous 2-D Linear System

The continuum limit of the equation of motion, (34), is the two-dimensional continuous lattice modeled by

$$\ddot{u} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}. \tag{37}$$

For the solution to (37), we look for an eigenfunction, $u_\lambda(x,y)$, which solves

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\lambda u \tag{38}$$

(a.k.a. an "eigensolution") and satisfies the boundary conditions

$$u(0,y) = u(L,y) = u(x,0) = u(x,L) = 0 \tag{39}$$

where L is the length of the lattice. We introduce the negative in (38) to match the system's negative, (11).

In one dimension, the solution to $u_{xx} = -\lambda u$, is $u(x) = A\sin(\alpha x) + B\cos(\beta x)$. We used the left boundary condition, $u(0) = 0 = A\sin(\alpha \cdot 0) + B\cos(\beta \cdot 0) = B$, to find that $B = 0$. Use that and the right side condition $u(L) = 0 = A\sin(\alpha L) + 0 \cdot \cos(\beta L) = A\sin(\alpha L)$ to find that $A\sin(\alpha L) = 0$. Since A and B can't both be 0, we have that $\alpha = {}^{k\pi}/_{L}$ $(k \in \mathbb{Z})$.

Returning to two dimensions, the eigenvector solutions to (38) will each be of the form

$$\begin{aligned} u_\lambda(x,y) = {} & A\sin(\alpha x)\sin(\beta y) + B\sin(\alpha x)\cos(\beta y) \\ & + C\cos(\alpha x)\sin(\beta y) + D\cos(\alpha x)\cos(\beta y) \end{aligned} \tag{40}$$

Using the boundary conditions, (39), in (40) yields the system

$$v_\lambda(0,y) = \qquad\qquad C\sin(\beta y) \qquad + D\cos(\beta y) \qquad = 0 \tag{41}$$

$$v_\lambda(L,y) = A\sin(\alpha L)\sin(\beta y) + B\sin(\alpha L)\cos(\beta y) + C\cos(\alpha L)\sin(\beta y) + D\cos(\alpha L)\cos(\beta y) = 0 \tag{42}$$

$$v_\lambda(x,0) = \qquad B\sin(\alpha x) \qquad + D\cos(\alpha x) \qquad = 0 \tag{43}$$

$$u_\lambda(x,L) = A\sin(\alpha x)\sin(\beta L) + B\sin(\alpha x)\cos(\beta L) + C\cos(\alpha x)\sin(\beta L) + D\cos(\alpha x)\cos(\beta L) = 0 \tag{44}$$

Factoring $\cos(\beta y)$ out of the second two terms in (42) leaves (41), which is zero, implying that

$$\begin{aligned} &A\sin(\alpha L)\sin(\beta y) + B\sin(\alpha L)\cos(\beta y) \\ &\quad = \sin(\alpha L)\Big(A\sin(\beta y) + B\cos(\beta y)\Big) = 0, \end{aligned}$$

from which we see that $\sin(\alpha L) = 0$, and thus $\alpha = \dfrac{j\pi}{L}$, (where $j \in \mathbb{Z}$).

Similarly, factoring $\cos(\beta L)$ out of the 2^{nd} and 4^{th} terms of (44) leaves (43), which equals zero, thus implying that

$$A\sin(\alpha x)\sin(\beta L) + C\cos(\alpha x)\sin(\beta L) \qquad = \sin(\beta L)\Big(A\sin(\alpha x) + C\cos(\alpha x)\Big) = 0,$$

which leads us to $\beta = \dfrac{k\pi}{L}$, (where $k \in \mathbb{Z}$).

Substitute α and β into a system of equations (41) through (44) to get

$$u_\lambda(0,y) = \qquad C\sin\left(\frac{k\pi}{L}y\right) + D\cos\left(\frac{k\pi}{L}y\right) = 0 \tag{45}$$

$$u_\lambda(L,y) = \qquad C\sin\left(\frac{k\pi}{L}y\right) + D\cos\left(\frac{k\pi}{L}y\right) = 0 \tag{46}$$

$$u_\lambda(x,0) = B\sin\left(\frac{j\pi}{L}x\right) \qquad + D\cos\left(\frac{j\pi}{L}x\right) = 0 \tag{47}$$

$$u_\lambda(x,L) = B\sin\left(\frac{j\pi}{L}x\right) \qquad + D\cos\left(\frac{j\pi}{L}x\right) = 0 \tag{48}$$

From (46) we see that $C = D = 0$. And from (48) we see that $B = D = 0$.

Therefore, only $A \neq 0$. For simplicity, we let $A = 1$. Then, for eigenvalue $\lambda_{j,k}$, we get the general eigensolution

$$u_{j,k}(x,y) = \sin\left(\frac{j\pi}{L}x\right)\sin\left(\frac{k\pi}{L}y\right). \tag{49}$$

Equation (49), then, is the eigensolution of (38) for eigenvalue $\lambda_{j,k}$ for the particle at position (x,y).

Check: Let $u = \sin\left(\frac{j\pi}{L}x\right)\sin\left(\frac{k\pi}{L}y\right)$, then

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -(j^2+k^2)\left(\frac{\pi}{L}\right)^2 \sin\left(\frac{j\pi}{L}x\right)\sin\left(\frac{k\pi}{L}y\right) = \lambda u,$$

where $\lambda = -(j^2+k^2)\left(\frac{\pi}{L}\right)^2$ is a scalar.

From the check, we can see that the corresponding eigenvalue is

$$\lambda_{j,k} = -(j^2+k^2)\left(\frac{\pi}{L}\right)^2.$$

Now to apply this to the discrete model.

3.2.2 Applying to the Discrete 2D Linear System

For the discrete $N \times N$ case, we have masses named with a double subscript, $M_{m,n}$ (where $m,n = 1,2,\ldots N$). The length, L, of the continuous system, is the same as the distance between masses, h, times the number of spaces, $N+1$, or $L = h(N+1)$. Mass m,n's horizontal position is $x = mh$, and it's vertical position is $y = nh$. So the first eigensolution, (49), becomes

$$\mathbf{v}_{j,k}(m,n) = \sin\left(\frac{jm\pi}{N+1}\right)\sin\left(\frac{kn\pi}{N+1}\right) \qquad (m,n = 1,2,\ldots N). \tag{50}$$

Equation (50) is one eigensolution to the two dimensional linear system. That is, for eigenvalue $\lambda_{j,k}$, it's corresponding eigenvector $\mathbf{v}_{j,k}$ is obtained by iterating m,n over $1,2,\ldots N$. The first, lowest frequency mode eigenvector, $\mathbf{v}_{1,1}$, is obtained by letting $j = k = 1$, is associated with $\lambda_{1,1}$, and is equivalent to the initial position, (35)

We check this solution in (34) (with $\beta = 0$) by first converting it to exponential form

$$\begin{aligned}
\mathbf{v}_{j,k}(m,n) &= \sin\left(\frac{j\pi m}{N+1}\right)\sin\left(\frac{k\pi n}{N+1}\right) \\
&= \frac{\omega^{jm}-\omega^{-jm}}{2i}\cdot\frac{\omega^{kn}-\omega^{-kn}}{2i} \\
&= -\frac{1}{4}\left(\omega^{jm+kn}-\omega^{jm-kn}-\omega^{-jm+kn}+\omega^{-jm-kn}\right), \qquad (51)
\end{aligned}$$

where $\omega = e^{\frac{i\pi}{N+1}}$.

We need to show that the last line of (51) solves (34), with $\beta = 0$. We start with the first term. Let $v_{m,n} = \omega^{jm+kn}$. Instead of the second derivative, as in the continuous model, we need to show that

$$v_{m-1,n} + v_{m+1,n} + v_{m,n-1} + v_{m,n+1} - 4v_{m,n} = -\lambda v_{m,n}.$$

Substitute for each of the vs and factor the left side

$$\begin{aligned}
&v_{m-1,n} + v_{m+1,n} + v_{m,n-1} + +v_{m,n+1} - 4v_{m,n} \\
&\quad = \omega^{j(m-1)+kn} + \omega^{j(m+1)+kn} + \omega^{jm+k(n-1)} + \omega^{jm+k(n+1)} - 4\omega^{jm+kn} \\
&\quad = \left(\omega^{-j} + \omega^{j} + \omega^{-k} + \omega^{k} - 4\right)\omega^{jm+kn}.
\end{aligned}$$

The expression in parenthesis does not depend on m or n, so it is a scalar multiple and, of course, ω^{jm+kn} is the original $v_{m,n}$. That is, the RHS is $-\lambda v_{m,n}$, with eigenvalue

$$\lambda_{j,k} = -\left(\omega^{-j} + \omega^{j} + \omega^{-k} + \omega^{k} - 4\right).$$

We have shown the first term of (51), ω^{jm+kn} is a solution. But since the other three terms are just different linear combinations of the same ω, they will all work out. Therefore, we have shown that (51) is a solution to (34) when $\beta = 0$.

Next we return the eigenvalue $\lambda_{j,k}$ back to trig functions:

$$\begin{aligned}\lambda_{j,k} &= -\left(\omega^{-j} + \omega^{j} + \omega^{-k} + \omega^{k} - 4\right) \\ &= -\left(e^{-i\frac{j\pi}{N+1}} + e^{i\frac{j\pi}{N+1}} + e^{-i\frac{k\pi}{N+1}} + e^{i\frac{k\pi}{N+1}} - 4\right) \\ &= 4 - 2\cos\left(\frac{j\pi}{N+1}\right) - 2\cos\left(\frac{k\pi}{N+1}\right). \end{aligned} \tag{52}$$

To summarize, eigenvalue $\lambda_{j,k}$ is given by (52), and it's corresponding eigenvector, given by (50), solves the linear version of (34) when $\beta = 0$.

We still need a final solution over time, analogous to (21), to compare to the numerical solution.

3.2.3 The Fourier Coefficients in Two Dimensions

The analog to (18) is

$$\begin{aligned}\mathbf{u}(t) &= \sum_{j=1}^{N}\sum_{k=1}^{N}\left[A_{j,k}\sin(\omega_{j,k}t) + B_{j,k}\cos(\omega_{j,k}t)\right]\mathbf{v}_{j,k} \\ &= \sum_{j=1}^{N}\sum_{k=1}^{N}\left[A_{j,k}\sin(\omega_{j,k}t) + B_{j,k}\cos(\omega_{j,k}t)\right]\sin\left(\frac{j\pi m}{N+1}\right)\sin\left(\frac{k\pi n}{N+1}\right), \end{aligned} \tag{53}$$

for $m,n = 1,2\ldots N$, where $\omega_{j,k} = \sqrt{\lambda_{j,k}}$.

For this work, all systems are started with zero velocity, or $\dot{\mathbf{u}}(0) = \mathbf{0}$, which gives

$$\begin{aligned}\dot{\mathbf{u}}(t) &= \sum_{j=1}^{N}\sum_{k=1}^{N}\left[A_{j,k}\omega_{j,k}\cos(\omega_{j,k}t) - B_{j,k}\omega_{j,k}\sin(\omega_{j,k}t)\right]\mathbf{v}_{j,k} \\ \dot{\mathbf{u}}(0) &= \sum_{j=1}^{N}\sum_{k=1}^{N}\left[A_{j,k}\omega_{j,k}\cos(\omega_{j,k}0) - B_{j,k}\omega_{j,k}\sin(\omega_{j,k}0)\right]\mathbf{v}_{j,k} \\ &= \sum_{j=1}^{N}\sum_{k=1}^{N}A_{j,k}\omega_{j,k}\mathbf{v}_{j,k} = \mathbf{0}. \end{aligned}$$

Therefore all $A_{j,k} = 0$. We can now reduce (53) to

$$\mathbf{u}(t) = \sum_{j=1}^{N} \sum_{k=1}^{N} B_{j,k} \cos(\omega_{j,k} t) \mathbf{v}_{j,k}. \tag{54}$$

For the initial position, we set $\mathbf{u}(0) = \mathbf{v}_{1,1}$. So, when $t = 0$, (54) becomes to

$$\mathbf{u}(0) = \sum_{j=1}^{N} \sum_{k=1}^{N} B_{j,k} \mathbf{v}_{j,k}$$

$$= \begin{pmatrix} \mathbf{v}_{1,1} \, \mathbf{v}_{1,2} \cdots \mathbf{v}_{1,N} \, \mathbf{v}_{2,1} \cdots \mathbf{v}_{N,N} \end{pmatrix} \begin{pmatrix} B_{1,1} \\ B_{1,2} \\ \vdots \\ B_{1,N} \\ B_{2,1} \\ \vdots \\ B_{N,N} \end{pmatrix} = \mathbf{v}_{1,1}.$$

Let $\mathbf{V} = \begin{pmatrix} \mathbf{v}_{1,1}, \, \mathbf{v}_{1,2}, \cdots \mathbf{v}_{1,N}, \, \mathbf{v}_{2,1}, \cdots \mathbf{v}_{N,N} \end{pmatrix}$ and note that it is the eigenvalues of a circulant matrix, therefore it is unitary (thus $\mathbf{V}^{-1} = \mathbf{V}^{\dagger}$), then we can solve for the Bs using

$$\mathbf{B} = \begin{pmatrix} B_{1,1} \\ B_{1,2} \\ \vdots \\ B_{1,N} \\ B_{2,1} \\ \vdots \\ B_{N,N} \end{pmatrix} = \mathbf{V}^{-1} \mathbf{v}_{1,1} = \mathbf{V}^{\dagger} \mathbf{v}_{1,1}$$

But since $\mathbf{V}$ is unitary, its columns are also orthogonal. That is, $\mathbf{v}_{l,m}^{\dagger} \mathbf{v}_{j,k} = 1$ whenever

$l = j$ and $m = k$, but $\mathbf{v}_{l,m}^{\dagger}\mathbf{v}_{j,k} = 0$ whenever $l \neq j$ or $m \neq k$. As a result, coefficient $B_{1,1} = 1$ and $B_{j,k} = 0$ otherwise. That is, only the coefficient associated with the initial condition eigenvector has any value.

So, finally, the solution to the linear 2 dimensional model, (54), can be reduced even further to

$$\mathbf{u}(t) = \cos(\sqrt{\lambda_{1,1}}t)\mathbf{v}_{1,1}. \tag{55}$$

We take the derivative with respect to time to find the solution for the velocities

$$\dot{\mathbf{u}}(t) = -\sqrt{\lambda_{1,1}}\sin(\sqrt{\lambda_{1,1}}t)\mathbf{v}_{1,1}. \tag{56}$$

Note that (55) and (56) are identical to (21) and (22), the solutions to the one dimensional linear system.

Equations (55) and (56) are used to test our code and our integrator (see section 6.2). We will use equations similar to (19) and (20), with the integrater's output (instead of the initial conditions) to find the Fourier coefficients, As and Bs, at any point in time during the simulation. But first we need to normalize the eigenvectors to create our transform matrix, $\mathbf{F}$.

3.2.4 Normalizing the 2-d Eigenvectors

We find the sum of the squares of eigenvector $\mathbf{v}_{j,k}$ of an $N \times N$ system. Each component of eigenvector $\mathbf{v}_{j,k}$ is given in (50). Writing that in exponential form, we get

$$\begin{aligned}
\mathbf{v}_{j,k} &= \sin\left(\frac{j\pi m}{N+1}\right) \cdot \sin\left(\frac{k\pi n}{N+1}\right) \\
&= \left(\frac{\omega^{jm} - \omega^{-jm}}{2i}\right)\left(\frac{\omega^{kn} - \omega^{-kn}}{2i}\right) \\
&= -\frac{1}{4}\left(\omega^{jm} - \omega^{-jm}\right)\left(\omega^{kn} - \omega^{-kn}\right),
\end{aligned}$$

where $\omega = e^{\frac{\pi}{N+1}i}$ and $m,n = 1,2,\ldots N$.

We sum the squares of the components. That is,

$$\begin{aligned}\sum_{m=1}^{N}\sum_{n=1}^{N}\mathbf{v}_{j,k}(m,n)^2 &= \sum_{m=1}^{N}\sum_{n=1}^{N}\left[-\frac{1}{4}\left(\omega^{jm}-\omega^{-jm}\right)\left(\omega^{kn}-\omega^{-kn}\right)\right]^2 \\ &= \frac{1}{16}\sum_{m=1}^{N}\sum_{n=1}^{N}\left(\omega^{2jm}-2+\omega^{-2jm}\right)\left(\omega^{2kn}-2+\omega^{-2kn}\right) \\ &= \frac{1}{16}\sum_{m=1}^{N}\left(\omega^{2jm}-2+\omega^{-2jm}\right)\cdot\sum_{n=1}^{N}\left(\omega^{2kn}-2+\omega^{-2kn}\right).\end{aligned}$$

Continuing with just the first summation, we eliminate the summation index, m, by recognizing the geometric series and recalling that $\omega^{N+1} = -1$

$$\begin{aligned}&\sum_{m=1}^{N}\left(\omega^{2jm}-2+\omega^{-2jm}\right) \\ &\quad= \sum_{m=1}^{N}\omega^{2jm}-\sum_{m=1}^{N}2+\sum_{m=1}^{N}\omega^{-2jm} \\ &\quad= \frac{\omega^{2j}-\omega^{2j(N+1)}}{1-\omega^{2j}}-2N+\frac{\omega^{-2j}-\omega^{-2j(N+1)}}{1-\omega^{-2j}} \\ &\quad= \frac{\omega^{2j}-1}{1-\omega^{2j}}-2N+\frac{\omega^{-2j}-1}{1-\omega^{-2j}} = -2-2N.\end{aligned}$$

We can do the same with the second summation, so we have

$$\sum_{m=1}^{N}\sum_{n=1}^{N}\mathbf{v}_{j,k}(m,n)^2 = \frac{1}{16}(-2-2N)^2 = \left(\frac{N+1}{2}\right)^2.$$

Finally, the magnitude of the eigenvectors is

$$\left\|\mathbf{v}_{j,k}(m,n)\right\| = \sqrt{\sum_{m=1}^{N}\sum_{n=1}^{N}\mathbf{v}_{j,k}(m,n)^2} = \frac{N+1}{2}.$$

Note that the magnitudes of all the eigenvectors are the same. We use this to create the two

dimension transform matrix, **F**, analog to (24),

$$\mathbf{F} = \frac{\mathbf{V}^{\dagger}}{\frac{N+1}{2}}. \tag{57}$$

3.3 Energy Calculations for the 2-D System

3.3.1 Show energy is conserved

Start with the Hamiltonian for the 2 dimensional system, from (33)

$$\begin{aligned} H = & \frac{1}{2}\sum_{m=0}^{N}\sum_{n=0}^{N}\left[\left(u_{m,n}-u_{m+1,n}\right)^2+\left(u_{m,n}-u_{m,n+1}\right)^2\right] \\ & +\frac{\beta}{4}\sum_{m=0}^{N}\sum_{n=0}^{N}\left[\left(u_{m,n}-u_{m+1,n}\right)^4+\left(u_{m,n}-u_{m,n+1}\right)^4\right] \\ & +\frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}\dot{u}_{m,n}^2. \end{aligned}$$

Take the derivative of it with respect to time

$$\begin{aligned} \dot{H} = & \sum_{m=0}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m+1,n}\right)\left(\dot{u}_{m,n}-\dot{u}_{m+1,n}\right) \\ & +\sum_{m=0}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m,n+1}\right)\left(\dot{u}_{m,n}-\dot{u}_{m,n+1}\right) \\ & +\beta\sum_{m=0}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m+1,n}\right)^3\left(\dot{u}_{m,n}-\dot{u}_{m+1,n}\right) \\ & +\beta\sum_{m=0}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m,n+1}\right)^3\left(\dot{u}_{m,n}-\dot{u}_{m,n+1}\right) \\ & +\sum_{m=1}^{N}\sum_{n=1}^{N}\dot{u}_{m,n}\ddot{u}_{m,n}. \end{aligned}$$

Distribute

$$\dot{H} = \sum_{m=0}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m+1,n}\right)\dot{u}_{m,n} - \sum_{n=0}^{N}\left(u_{m,n}-u_{m+1,n}\right)\dot{u}_{m+1,n}$$

$$
\begin{aligned}
&+\sum_{m=0}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m,n+1}\right)\dot{u}_{m,n}-\sum_{m=0}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m,n+1}\right)\dot{u}_{m,n+1}\\
&+\beta\sum_{m=0}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m+1,n}\right)^{3}\dot{u}_{m,n}-\beta\sum_{m=0}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m+1,n}\right)^{3}\dot{u}_{m+1,n}\\
&+\beta\sum_{m=0}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m,n+1}\right)^{3}\dot{u}_{m,n}-\beta\sum_{m=0}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m,n+1}\right)^{3}\dot{u}_{m,n+1}\\
&+\sum_{m=1}^{N}\sum_{n=1}^{N}\dot{u}_{m,n}\ddot{u}_{m,n}.
\end{aligned}
$$

Note that $\dot{u}_{0,n}=\dot{u}_{m,0}=0$, so that we can eliminate many of the zero indices

$$
\begin{aligned}
\dot{H}=&\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m,n}-u_{m+1,n}\right)\dot{u}_{m,n}-\sum_{m=0}^{N}\sum_{n=1}^{N}\left(u_{m,n}-u_{m+1,n}\right)\dot{u}_{m+1,n}\\
&+\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m,n}-u_{m,n+1}\right)\dot{u}_{m,n}-\sum_{m=1}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m,n+1}\right)\dot{u}_{m,n+1}\\
&+\beta\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m,n}-u_{m+1,n}\right)^{3}\dot{u}_{m,n}-\beta\sum_{m=0}^{N}\sum_{n=1}^{N}\left(u_{m,n}-u_{m+1,n}\right)^{3}\dot{u}_{m+1,n}\\
&+\beta\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m,n}-u_{m,n+1}\right)^{3}\dot{u}_{m,n}-\beta\sum_{m=1}^{N}\sum_{n=0}^{N}\left(u_{m,n}-u_{m,n+1}\right)^{3}\dot{u}_{m,n+1}\\
&+\sum_{m=1}^{N}\sum_{n=1}^{N}\dot{u}_{m,n}\ddot{u}_{m,n}.
\end{aligned}
$$

Shift the remaining zero indices to start at 1, and note that $\dot{u}_{0,N+1}=\dot{u}_{N+1,0}=0$, thereby eliminating the $N+1$ from those indices

$$
\begin{aligned}
\dot{H}=&\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m,n}-u_{m+1,n}\right)\dot{u}_{m,n}-\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m-1,n}-u_{m,n}\right)\dot{u}_{m,n}\\
&+\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m,n}-u_{m,n+1}\right)\dot{u}_{m,n}-\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m,n-1}-u_{m,n}\right)\dot{u}_{m,n}\\
&+\beta\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m,n}-u_{m+1,n}\right)^{3}\dot{u}_{m,n}-\beta\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m-1,n}-u_{m,n}\right)^{3}\dot{u}_{m,n}\\
&+\beta\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m,n}-u_{m,n+1}\right)^{3}\dot{u}_{m,n}-\beta\sum_{m=1}^{N}\sum_{n=1}^{N}\left(u_{m,n-1}-u_{m,n}\right)^{3}\dot{u}_{m,n}\\
&+\sum_{m=1}^{N}\sum_{n=1}^{N}\dot{u}_{m,n}\ddot{u}_{m,n}.
\end{aligned}
$$

Finally, factor out $\dot{u}_{m,n}$, leaving the equation of motion, (34), which equals zero,

$$\begin{aligned}
\dot{H} = &- \sum_{m=1}^{N} \sum_{n=1}^{N} \Big[\left(u_{m-1,n} - u_{m,n}\right) + \left(u_{m+1,n} - u_{m,n}\right) \\
&+ \left(u_{m,n-1} - u_{m,n}\right) + \left(u_{m,n+1} - u_{m,n}\right) \\
&+ \beta \Big(\left(u_{m-1,n} - u_{m,n}\right)^3 + \left(u_{m+1,n} - u_{m,n}\right)^3 \\
&+ \left(u_{m,n-1} - u_{m,n}\right)^3 + \left(u_{m,n+1} - u_{m,n}\right)^3 \Big) \\
&+ \ddot{u}_{m,n} \Big] \dot{u}_{m,n} \\
= &- \sum_{m=1}^{N} \sum_{n=1}^{N} 0 \cdot \dot{u}_{m,n} = 0,
\end{aligned}$$

thereby proving that the Hamiltonian has constant energy (i.e., that it is, in fact, a Hamiltonian).

3.3.2 Initial Energy in the 2D Model

Since the system starts at rest, there is no kinetic energy. To calculate the value of energy, we use the two dimension's initial conditionfrom (35) in exponential form

$$\begin{aligned}
8u_{m,n}(0) &= \sin\left(\frac{m\pi}{N+1}\right) \sin\left(\frac{n\pi}{N+1}\right) \\
&= -\frac{1}{4}\left(\omega^{m+n} - \omega^{m-n} - \omega^{-m+n} + \omega^{-m-n}\right),
\end{aligned}$$

where $\omega = e^{\frac{i\pi}{N+1}}$. We substitute that into the potential energy, from (32)

$$\begin{aligned}
U(\mathbf{u}) = &\frac{1}{32} \sum_{m=0}^{N} \sum_{n=0}^{N} \left[\left(u_{m,n} - u_{m+1,n}\right)^2 + \left(u_{m,n} - u_{m,n+1}\right)^2 \right] \\
&+ \frac{\beta}{64} \sum_{m=0}^{N} \sum_{n=0}^{N} \left[\left(u_{m,n} - u_{m+1,n}\right)^4 + \left(u_{m,n} - u_{m,n+1}\right)^4 \right].
\end{aligned}$$

It is clear that this is too much to do by hand. For this research, we plugged this into Maple and compared the answer to the energy level calculated from the actual results (see

section 6.2).

4 Fourier Modes

The physical state of an FPU system can be entirely described by each masses' position and velocity. The position and velocity data can each be compared to the normal modes, based on the eigenvalues of the linear system's matrix. In a finite 1 dimensional system, there are only a finite number of these component frequencies, equal to the number of masses. Thus, we can break the energy configuration of the system down into a finite number of modes, and plot the energy in each mode over time (e.g., figure 2).

From the derivation of the transform matrix **F**, (24), we find the energy in each mode by first converting the integrator's position and velocity data output to Fourier space

$$\mathbf{w}_j = \mathbf{v}_j^\dagger \dot{\mathbf{u}}$$
$$\dot{\mathbf{w}}_j = \mathbf{v}_j^\dagger \mathbf{u},$$

respectively, where λ_j is the j^{th} eigenvalue of the matrix formed by the linear system, and $\mathbf{v}_j$, the normalized j^{th} eigenvector, is

$$\mathbf{v}_j(n) = \frac{\sin\left(\frac{j\pi n}{N+1}\right)}{\sqrt{\frac{N+1}{2}}} \qquad (n = 1 \ldots N).$$

This is implemented in matrix **F**, (24). Then the kinetic and potential energy in mode j comes from (25), is

$$H_j = \frac{1}{2}\mathbf{w}_j^\intercal \lambda_j \mathbf{w}_j + \frac{1}{2}\dot{\mathbf{w}}_j^\intercal \dot{\mathbf{w}}_j.$$

The two dimension equations are the same (not counting the subscripts),

$$\mathbf{w}_{j,k} = \mathbf{v}_{j,k}^{\dagger}\mathbf{u}$$
$$\dot{\mathbf{w}}_{j,k} = \mathbf{v}_{j,k}^{\dagger}\dot{\mathbf{u}},$$

except that the normalized eigenvectors are

$$\mathbf{v}_{j,k}(m,n) = \frac{\sin\left(\frac{j\pi m}{N+1}\right)\sin\left(\frac{k\pi n}{N+1}\right)}{\left(\frac{N+1}{2}\right)} \qquad (m,n = 1\ldots N).$$

This is implemented in the 2D matrix **F**, (57). Then the energy in mode j,k is given by

$$H_{j,k} = \frac{1}{2}\mathbf{w}_{j,k}^{\mathsf{T}}\lambda_{j,k}\mathbf{w}_{j,k} + \frac{1}{2}\dot{\mathbf{w}}_{j,k}^{\mathsf{T}}\dot{\mathbf{w}}_{j,k}.$$

In other words, for both one and two dimensions, we find the energy in the modes at any point in time by left multiplying matrix **F** (equations (24) and (57)) by the position and velocity of the modes at that time, and then applying (25) to the result.

5 Equipartition (or Thermalization)

The state of having the energy equally divided among the Fourier modes is known as *equipartition*. It is analogous to the state of thermal equilibrium in a gas and in statistical mechanics it is known as the *equipartition theorem*. Without this theorem, statistical mechanics can not be extended to thermodynamics on the macroscopic level [6] and our real world experience, e.g. heat expanding to fill an entire room, would not exist.

Before FPU, scientists believed that nonlinearity was enough to ensure equipartition. If equipartition could not be assumed, then the entire basis of thermodynamics could be called into question and raises the question of what does cause equipartition.

5.1 Partial Resolution

In 1967, Norman J. Zabusky and Gary Deem found that FPU systems would reach equipartition if only they had enough initial energy. FPU had simply started their system with too little energy to reach equipartition [6].

Later research by Eddie Cohen has shown that the FPU recurrences only occur if the total energy per oscillator, (known as the *specific energy*), in the system is below a certain threshold. Above the threshold, the system enters equipartition. Cohen also found that increasing the number of masses reduces the per oscillator threshold. In other words, as the system size increases, it's easier for the system to thermalize. In a system with infintely many masses — like the real world — the system thermalizes for any level of energy [6, p. 220]. This conforms with what we observe in everyday life.

In 1972, James Tuck and Mary Tsingou-Menzel[4] conducted extensive numerical simulations and put to rest any concern that FPU's recurrences were a result of not running the simulation long enough. They also found that the system experiences even stronger recurrences over even longer time periods, called "superrecurrences" [6, p. 216].

Once it was determined that the system acts as expected for real-world situations, the scientific community seems to have breathed a sigh of relief and forgotten about the issue entirely — there is no mention of it in published work [3].

But we still don't know why the recurrences occur in the first place. This work shows that they do not occur in two dimensions.

6 The Systems

We simulated the FPU β, or cubic, model in one dimension using the system and initial conditions described in section 2, equations (1), (2) and (3).

We ran one dimensional systems with $N = 8$ and $N = 8^2 = 64$ masses and with $N = 32$

[4]The original FPU programmer, using her married name.

and $N = 32^2 = 1024$. As stated, we always started the systems at rest and all the energy in the first mode. We tested systems varying β over the integers $1, 2 \ldots 32$. We converted the data to Fourier space using using the transform matrix, **F**, equation (24), derived in section 2.2.4, as

$$\mathbf{w} = \mathbf{F}\mathbf{u}.$$

And finally, calculated the potential and kinetic energy, respectively, in each mode using (25) as follows

$$U_j = \frac{1}{2}\mathbf{w}^\mathsf{T} D\mathbf{w}$$
$$T_j = \frac{1}{2}\dot{\mathbf{w}}^\mathsf{T}\dot{\mathbf{w}}$$

We graph the lowest few modes of these equations to see how much energy is in each. The energy will start completely in the first mode. If the system experiences recurrences like the ones FPU saw, the energy will leave the first mode, and then nearly all will return to the first mode.

We ran the two dimension FPU β model, using the system and initial position described in section section 3.1, equations (33), (34) and (35). We use the same equations as above to transform the output to Fourier space and calculate the energy in each mode, but replace **F** with (57), from section 3.2.4.

In two dimensions, we ran square models of size $N \times N = 8 \times 8$, to compare to the straight 8 and 64 models, and of size $N \times N = 32 \times 32$, to compare to the straight 32 and 1024 models, varying β from $1 \ldots 32$. We referred to the straight 8 and 64, and the 2 dimension 8×8 systems as the "Eight Models", and the straight 32 and 1024 and 2 dimension 32×32 systems as the "Thirty-two Models".

6.1 Implementation

The system was implemented in C on Linux, using SUNDIALS' CVODE initial value ODE solver [5] using the Backwards Differentiation solver and Newton iteration. We analyzed the output using GNU Octave. For completeness, the entire code is available by contacting David Trubatch at Montclair State University[5].

6.2 Validation

In one dimension, with $\beta = 0$, we have a linear system which has (21) and (22) as the exact solution. In two dimensions, the exact solutions is (55) and (56). We simulated the linear systems and compared the output to the exact solution. Our results are given in table 3 and 4. Note that as the tolerance gets smaller, the difference between the integrator's solution and the exact solution also shrinks. This indicates that the integrator is working and that we have configured it and are using it correctly.

We also did the above with different initial conditions (e.g., starting in different modes, starting with combinations of modes) and compared them to the exact solutions, with similar results (not shown).

To check that our equations were correct, we calculated the energy in the linear models at every time unit (which we called a "second") in both Euclidean and Fourier space and compared the difference. These results are in tables 5 and 6. Notice that the last column, titled *Difference*, is small.

But we can't verify the integrator's results for the nonlinear systems by comparison to an exact solution, because none exists (if there were, we would have nothing to research), or by calculating the energy in Fourier space. We validated these systems using two methods. First, we calculated the energy's system at each second from the integrator's position and velocity output to be sure it had not lost too much energy. And second, we ran the systems backwards, using the forward simulation's last condition as the reverse simulation's initial

[5] `http://www.montclair.edu/profilepages/view_profile.php?username=trubatchd`

condition, to see if it returned to the initial condition.

To calculate the energy at each second, we first calculated the initial energy, using the initial conditions and equation (31) for one dimension and Maple's results from section 3.3.2 for two dimensions and compared that to a calculation of the energy at $t = 0$ of the systems. Then we simply used the Hamiltonians — equations (1) and (33) – and the integrator's position and velocity output to calculate the energy at each second for duration of the simulation. For each value of β, we calculated the difference of the maximum and minimum energy divided by the initial energy. Our results are in the last columns of tables 7 through 12.

Finally, we verified our code by running the systems backwards to see if they returned to their initial condition. To find the equation of motion for the backwards system, we first note that the equation of motion, (2), has an implicit variable for time in it. Including this variable, it becomes (we will deal with just the linear model for the moment)

$$\ddot{u}_n(t) = u_{n-1}(t) - 2u_n(t) - u_{n+1}(t).$$

Using the first order equations, (12), that is

$$\dot{u}_n(t) = v_n(t)$$
$$\dot{v}_n(t) = u_{n-1}(t) - 2u_n(t) + u_{n+1}(t).$$

We create a new variable, let $\tau = t_F - t$, where t_F represents the length of the simulation, and write the system with respect to τ

$$\dot{u}_n(\tau) = v_n(\tau)$$
$$\dot{v}_n(\tau) = u_{n-1}(\tau) - 2u_n(\tau) + u_{n+1}(\tau).$$

Note that "dot notation", $\dot{u}_n$, means the derivative with respect to time, t, not τ (even after

we've rewritten it). So by the chain rule, the left side of the system is really

$$\frac{\mathrm{d}\big(u_n(\tau)\big)}{\mathrm{d}t} = \frac{\mathrm{d}\big(u_n(\tau)\big)}{\mathrm{d}\tau}\frac{\mathrm{d}\tau}{\mathrm{d}t} = -\frac{\mathrm{d}\big(u_n(\tau)\big)}{\mathrm{d}\tau}$$
$$\frac{\mathrm{d}\big(v_n(\tau)\big)}{\mathrm{d}t} = \frac{\mathrm{d}\big(v_n(\tau)\big)}{\mathrm{d}\tau}\frac{\mathrm{d}\tau}{\mathrm{d}t} = -\frac{\mathrm{d}\big(v_n(\tau)\big)}{\mathrm{d}\tau}$$

because $\frac{\mathrm{d}\tau}{\mathrm{d}t} = -1$.

Put that back into the left side of the system, multiply both sides (of both equations) by -1 and rename τ back to t and we get

$$\dot{u}_n(t) = -v_n(t)$$
$$\dot{v}_n(t) = -\left(u_{n-1}(t) - 2u_n(t) + u_{n+1}(t)\right).$$

This says that to run the system backwards, just negate the function fed into the integrator.

This result is the same if we had used the nonlinear model or done it for the two dimensional system. That is, to run the one dimension β system backwards, we need to program the right side as

$$\dot{u}_n(t) = -v_n(t)$$
$$\dot{v}_n(t) = -\left(u_{n-1}(t) - 2u_n(t) + u_{n+1}(t) + \beta\left[(u_{n-1} - u_n)^3 - (u_n - u_{n+1})^3\right]\right).$$

And for the two dimension β system, we program

$$\begin{aligned}
\dot{u}_{m,n}(t) &= -\left(v_{m,n}(t)\right) \\
\dot{v}_{m,n}(t) &= -\Big[\big[(u_{m-1,n}(t) - u_{m,n}(t)) + (u_{m+1,n}(t) - u_{m,n}(t)) \\
&\qquad + (u_{m,n-1}(t) - u_{m,n}(t)) + (u_{m,n+1}(t) - u_{m,n}(t))\big] \\
&\quad + \beta\Big[(u_{m-1,n}(t) - u_{m,n}(t))^3 + (u_{m+1,n}(t) - u_{m,n}(t))^3 \\
&\qquad + (u_{m,n-1}(t) - u_{m,n}(t))^3 + (u_{m,n+1}(t) - u_{m,n}(t))^3\Big]\Big]
\end{aligned}$$

to run it backwards.

We programmed that as the right hand side to send to the integrator. For the initial conditions, we used the forward simulation's conditions — the masses' positions and velocities — at various times, which we called the forward's last condition. For example, if we used the forward system's condition at $t = 100$ seconds, we considered that as the forward's last condition, and fed it into the reverse simulation code, which would then run for 100 seconds, bringing us back to $t = 0$.

We then compared the forward simulation's initial condition (at $t = 0$) and the backward simulation's last condition (also at $t = 0$) by calculating the energy in the difference of the two positions. That is, we found the difference of mass n's position and velocity and fed those differences into the Hamiltonian. We call this output the "Delta Energy".

We ran the systems backwards for time units of $t = 10000$, 20000, 30000, and 40000 seconds. Our results are in tables 13 through 18.

6.3 Valid Simulations

We considered a system simulation valid if it's energy variation (maximum minus minimum) over 40000 seconds varied by less than 5% of the initial energy, and the energy difference at $t = 0$ between the reverse execution's last condition and the forward's initial conditions was less than 5% of the forward's initial condition.

We had to discard all of the Eight models (see Table 1) because the straight 8 mass systems and the square 8×8 mass systems did not return to the original energy configuration when run backwards. The straight 64 mass systems had satisfactory results (and had recurrence for $\beta = 4 \ldots 12$). But since none of the other Eight models were valid, we had nothing to compare the straight 64 mass systems to.

We also discarded straight 32 mass systems (see Table 2) for $\beta \geq 9$ and the 32×32 mass systems for $\beta \geq 22$ because they did not return to the original energy configuration.

7 Results

That leaves the usable systems as the straight $N = 32$ systems for $\beta = 1 \ldots 8$, the straight 1024 mass systems for any β, and the square 32×32 systems for $\beta = 1 \ldots 21$. The following results are summarized in Tables 1 and 2.

For the one dimension model, $N = 32$ mass system we found the recurrence to occur for $\beta = 5 \ldots 8$ (e.g., see Figure 2a). Note that this is nearly a duplicate of the original FPU model, and the energy graph matches the original [4]. For $\beta = 7, 8$, the system thermalized after one or more recurrences (see Figure 2b).

However, for the system with $N = 32^2 = 1024$ masses acted like a near-linear system — the energy in mode 1 fluctuated, but was never shared with other modes in any significant amount.

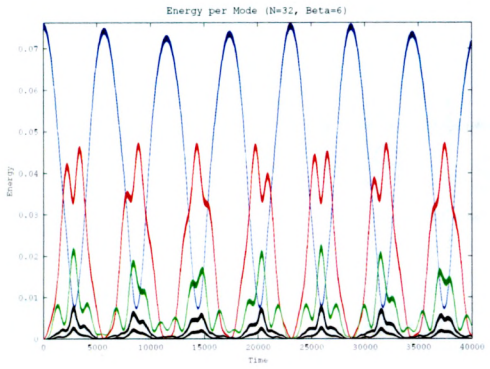
We could not find a recurrence zone in the 2-dimensional, $N \times N = 32 \times 32$ mass system. For $\beta = 1 \ldots 15$, the energy in the lowest modes never shared energy at all (see Figure 2c). For $\beta = 16 \ldots 32$, the system broke down into a thermalized state after several oscillations (see Figure 2d).

An interesting side note is that the system seems to behave better as you add more masses. We are unable to clearly explain why this is.

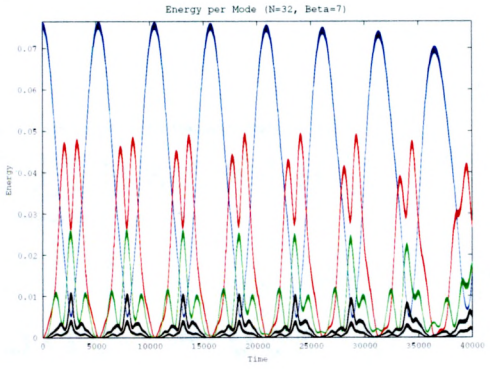
Our results are summarized in tables 1 and 2.

Table 1: Summary of Results: "Eight" Models

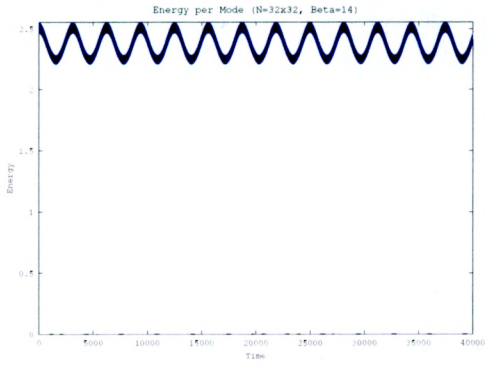
System	**8**	**64**	**8 × 8**
Energy Conserved	All β	$\beta \leq 23$	All β
$\Delta H = 0$ at $t = 0$	$\beta = 1$	$\beta \leq 30$	None
Recurrence	—	$\beta = 4 \ldots 13$	—
Thermalizes	—	$\beta \geq 14$	—



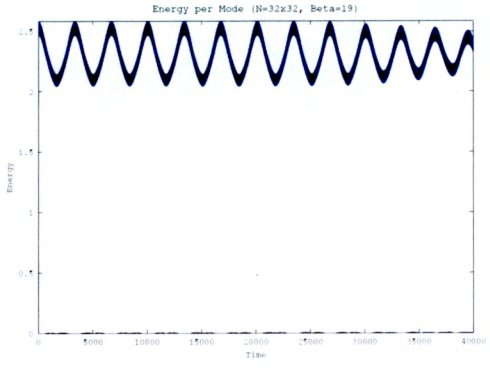
(a) $N = 32, \beta = 6$ recurrent system.



(b) $N = 32, \beta = 7$ recurrent system.



(c) $N = 32 \times 32, \beta = 14$.



(d) $N = 32 \times 32, \beta = 19$.

Figure 2: Energy per mode of various systems. Blue is the energy in Mode 1. Red is Mode 2. Green Mode 3.

Table 2: Summary of Results: "Thirty-two" Models

System	**32**	**1024**	**32×32**
Energy Conserved	$\beta \leq 13$	All β	$\beta \leq 21$
$\Delta H = 0$ at $t = 0$	$\beta \leq 8$	All β	$\beta \leq 21$
Recurrence	$\beta = 6 \ldots 8$	Acts linear	None
Thermalizes	$\beta \geq 7$	None	None

8 Conclusion

The straight 32 mass systems (Figure 2a) show the well-known FPU recurrence. But we could not find any recurrence in the larger 1024 mass system. In fact, the straight 1024 mass system acted like a linear system, never losing an significant amount of energy from the first mode. We originally thought this had something to do with scaling, but could not find an adequate scaling.

The 2 dimensional system with the same number masses (see figures 2c and 2d) showed little energy sharing. The energy in the first mode oscillated within a 10% range of its initial, but never completely lost it's energy, and they never reached equipartition.

We did not any results from our "Eight" model simulations due accuracy issues with our numerical scheme.

9 Next Steps

We would like to resolve the numerical issues which caused most of the "Eight" models to lose energy or fail to return to the original state when run backwards.

We attempted to determine how to scale the system so that different size systems and different dimensions look the same, but were unable to find an adequate scaling. We would like to understand how to scale these systems in one and two dimensions.

References

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A Tables

1 Dimensional Linear ($\beta = 0$)

At tolerance...	**...the maximum of |exact solution − numerical solution| is...**					
Tolerance	4 Masses		8 Masses		16 Masses	
	U	$\dot{U}$	U	$\dot{U}$	U	$\dot{U}$
1.00E-02	2.79E+00	9.31E-01	3.08E+00	2.96E+02	1.77E-01	2.23E+03
1.00E-03	2.79E+00	5.44E+00	3.08E+00	6.11E+00	1.77E-01	3.48E-02
1.00E-04	1.83E-01	3.18E-01	2.21E-01	4.27E-01	1.98E-01	3.91E-01
1.00E-05	1.09E-03	8.25E-04	3.59E-04	5.39E-04	2.19E-02	4.25E-02
1.00E-06	7.46E-04	5.02E-04	6.34E-05	4.63E-05	1.72E-03	3.37E-03
1.00E-07	1.27E-05	1.23E-05	1.94E-05	7.44E-06	4.70E-05	5.26E-05
1.00E-08	1.26E-05	7.97E-06	4.48E-07	6.42E-07	6.48E-07	3.15E-07
1.00E-09	1.04E-05	6.57E-06	1.93E-07	8.65E-08	5.63E-08	1.04E-07
1.00E-10	1.45E-06	9.13E-07	8.16E-10	1.27E-09	4.61E-09	5.42E-09
1.00E-11	2.02E-07	1.27E-07	3.64E-10	2.54E-10	2.06E-09	9.34E-10
1.00E-12	1.46E-09	9.18E-10	1.10E-08	3.80E-09	4.32E-09	8.03E-10
1.00E-13	7.87E-10	4.95E-10	1.19E-10	4.85E-11	5.02E-11	1.29E-11
1.00E-14	3.17E-10	1.91E-10	2.16E-12	9.25E-13	8.72E-12	1.72E-12

At tolerance...	**...the maximum of |exact solution − numerical solution| is...**					
Tolerance	32 Masses		64 Masses		128 Masses	
	U	$\dot{U}$	U	$\dot{U}$	U	$\dot{U}$
1.00E-02	1.24E-01	1.55E-01	1.40E-02	2.20E+01	1.46E-02	4.67E+02
1.00E-03	1.24E-01	2.07E-01	1.40E-02	8.53E-03	1.46E-02	1.23E-02
1.00E-04	4.09E-02	6.00E-02	2.03E-01	4.03E-01	6.89E-01	1.36E+00
1.00E-05	4.00E-02	7.98E-02	1.43E-02	2.63E-02	5.73E-02	1.14E-01
1.00E-06	2.00E-03	3.94E-03	3.49E-03	6.98E-03	3.34E-03	6.65E-03
1.00E-07	1.63E-04	3.22E-04	4.45E-04	8.78E-04	2.05E-04	4.04E-04
1.00E-08	6.58E-07	4.60E-07	4.49E-05	8.55E-05	7.82E-05	1.55E-04
1.00E-09	1.32E-06	1.90E-06	2.07E-06	4.06E-06	3.19E-06	6.34E-06
1.00E-10	4.16E-09	6.79E-09	2.59E-07	4.61E-07	2.76E-07	5.54E-07
1.00E-11	4.09E-10	4.51E-10	1.97E-10	2.86E-10	2.09E-08	4.10E-08
1.00E-12	4.52E-11	4.30E-11	1.60E-11	2.31E-11	2.79E-10	1.34E-10
1.00E-13	3.12E-11	9.38E-12	6.51E-12	4.44E-12	7.61E-12	2.88E-12
1.00E-14	7.14E-12	1.00E-12	2.87E-12	3.27E-13	1.07E-11	7.00E-13

Note: IC all in mode 1, no velocity, for 1000 time units with output every 1 unit.

Table 3: Comparison of integrator's output of 1 dimension linear ($\beta = 0$) system to the exact solution.

2 Dimensional Linear ($\beta = 0$)

At tolerance...	**...the maximum of |exact solution − numerical solution| is...**					
Tolerance	4×4 Masses		8×8 Masses		16×16 Masses	
	U	$\dot{U}$	U	$\dot{U}$	U	$\dot{U}$
1.00E-04	3.16E-01	8.02E-01	1.30E-01	3.44E-01	2.63E-01	7.33E-01
1.00E-05	2.87E-02	2.50E-02	1.76E-02	4.96E-02	4.23E-02	1.17E-01
1.00E-06	2.20E-03	1.91E-03	7.46E-05	8.47E-05	3.92E-05	7.08E-05
1.00E-07	8.10E-06	1.09E-05	3.61E-05	2.03E-05	2.62E-04	6.98E-04
1.00E-08	1.57E-05	1.39E-05	4.37E-07	5.57E-07	8.87E-07	3.93E-07
1.00E-09	1.65E-05	1.45E-05	1.16E-07	8.05E-08	4.89E-08	1.24E-07
1.00E-10	2.31E-06	2.02E-06	1.42E-09	2.83E-09	5.90E-09	1.04E-08
1.00E-11	3.19E-07	2.78E-07	2.91E-10	3.40E-10	2.70E-09	1.34E-09
1.00E-12	2.24E-09	1.94E-09	1.45E-08	7.17E-09	1.07E-09	2.88E-10
1.00E-13	1.28E-09	1.11E-09	5.29E-10	2.60E-10	7.62E-11	2.38E-11

At tolerance...	**...the maximum of |exact solution − numerical solution| is...**			
Tolerance	32×32 Masses		64×64 Masses	
	U	$\dot{U}$	U	$\dot{U}$
1.00E-04	7.68E-02	1.67E-01	6.37E-03	1.27E-03
1.00E-05	6.67E-02	1.88E-01	5.65E-03	8.77E-03
1.00E-06	1.14E-03	3.17E-03	3.94E-03	1.11E-02
1.00E-07	3.12E-04	8.84E-04	2.49E-04	7.23E-04
1.00E-08	2.91E-05	7.93E-05	1.07E-05	2.94E-05
1.00E-09	1.98E-06	4.76E-06	4.24E-06	1.16E-05
1.00E-10	1.37E-09	3.36E-09	5.56E-07	1.51E-06
1.00E-11	7.14E-10	1.51E-09	1.57E-10	3.20E-10
1.00E-12	5.60E-11	6.28E-11	2.46E-11	6.91E-11
1.00E-13	2.09E-11	1.69E-11	9.74E-12	6.89E-12

Note: IC all in mode 1, no velocity, for 1000 time units with output every 1 unit.

Table 4: Comparison of integrator's output of 2 dimension linear ($\beta = 0$) system to the exact solution.

Total Energy in 1 Dimensional Linear ($\beta = 0$) Model

		Physical Space					Fourier Space				
N	Tolerance	Initial	Min	Max	Range (Abs.)	Range (Rel.)	Min	Max	Range (Abs.)	Range (Rel.)	Difference
4	1.00E-04	0.95	0.95	1.25	2.94E-01	3.08E-01	0.95	1.25	2.94E-01	3.08E-01	1.00E-15
	1.00E-05	0.95	0.95	0.96	1.79E-03	1.88E-03	0.95	0.96	1.79E-03	1.88E-03	1.00E-15
	1.00E-06	0.95	0.95	0.95	1.30E-03	1.36E-03	0.95	0.95	1.30E-03	1.36E-03	1.00E-15
	1.00E-07	0.95	0.95	0.95	1.00E-05	1.05E-05	0.95	0.95	1.00E-05	1.05E-05	1.00E-15
	1.00E-08	0.95	0.95	0.95	1.03E-05	1.08E-05	0.95	0.95	1.03E-05	1.08E-05	1.00E-15
	1.00E-09	0.95	0.95	0.95	2.13E-05	2.23E-05	0.95	0.95	2.13E-05	2.23E-05	1.00E-15
	1.00E-10	0.95	0.95	0.95	2.97E-06	3.11E-06	0.95	0.95	2.97E-06	3.11E-06	1.00E-15
	1.00E-11	0.95	0.95	0.95	4.14E-07	4.33E-07	0.95	0.95	4.14E-07	4.33E-07	1.00E-15
	1.00E-12	0.95	0.95	0.95	2.45E-09	2.56E-09	0.95	0.95	2.45E-09	2.56E-09	1.00E-15
	1.00E-13	0.95	0.95	0.95	1.58E-09	1.66E-09	0.95	0.95	1.58E-09	1.66E-09	1.00E-15
	1.00E-14	0.95	0.95	0.95	1.21E-10	1.27E-10	0.95	0.95	1.21E-10	1.27E-10	1.00E-15
8	1.00E-04	0.54	0.54	1.40	8.60E-01	1.59E+00	0.54	1.40	8.60E-01	1.59E+00	2.00E-15
	1.00E-05	0.54	0.54	0.54	9.45E-05	1.74E-04	0.54	0.54	9.45E-05	1.74E-04	1.00E-15
	1.00E-06	0.54	0.54	0.54	5.24E-05	9.66E-05	0.54	0.54	5.24E-05	9.66E-05	1.00E-15
	1.00E-07	0.54	0.54	0.54	2.02E-05	3.73E-05	0.54	0.54	2.02E-05	3.73E-05	1.00E-15
	1.00E-08	0.54	0.54	0.54	1.07E-07	1.97E-07	0.54	0.54	1.07E-07	1.97E-07	1.00E-15
	1.00E-09	0.54	0.54	0.54	4.71E-08	8.68E-08	0.54	0.54	4.71E-08	8.68E-08	1.00E-15
	1.00E-10	0.54	0.54	0.54	6.17E-10	1.14E-09	0.54	0.54	6.17E-10	1.14E-09	1.00E-15
	1.00E-11	0.54	0.54	0.54	3.62E-10	6.67E-10	0.54	0.54	3.62E-10	6.67E-10	1.00E-15
	1.00E-12	0.54	0.54	0.54	7.63E-10	1.41E-09	0.54	0.54	7.63E-10	1.41E-09	1.00E-15
	1.00E-13	0.54	0.54	0.54	3.82E-13	7.04E-13	0.54	0.54	3.83E-13	7.05E-13	1.00E-15
	1.00E-14	0.54	0.54	0.54	1.31E-12	2.42E-12	0.54	0.54	1.31E-12	2.42E-12	1.00E-15
16	1.00E-04	0.29	0.29	1.33	1.04E+00	3.59E+00	0.29	1.33	1.04E+00	3.59E+00	4.00E-15
	1.00E-05	0.29	0.29	0.30	1.03E-02	3.57E-02	0.29	0.30	1.03E-02	3.57E-02	2.00E-15
	1.00E-06	0.29	0.29	0.29	9.67E-05	3.34E-04	0.29	0.29	9.67E-05	3.34E-04	3.00E-15
	1.00E-07	0.29	0.29	0.29	3.72E-06	1.28E-05	0.29	0.29	3.72E-06	1.28E-05	2.00E-15
	1.00E-08	0.29	0.29	0.29	3.61E-07	1.25E-06	0.29	0.29	3.61E-07	1.25E-06	3.00E-15
	1.00E-09	0.29	0.29	0.29	3.52E-09	1.22E-08	0.29	0.29	3.52E-09	1.22E-08	3.00E-15
	1.00E-10	0.29	0.29	0.29	3.68E-10	1.27E-09	0.29	0.29	3.68E-10	1.27E-09	2.00E-15
	1.00E-11	0.29	0.29	0.29	1.41E-10	4.86E-10	0.29	0.29	1.41E-10	4.86E-10	3.00E-15
	1.00E-12	0.29	0.29	0.29	1.83E-10	6.31E-10	0.29	0.29	1.83E-10	6.31E-10	2.00E-15
	1.00E-13	0.29	0.29	0.29	3.85E-12	1.33E-11	0.29	0.29	3.85E-12	1.33E-11	3.00E-15
	1.00E-14	0.29	0.29	0.29	3.19E-12	1.10E-11	0.29	0.29	3.19E-12	1.10E-11	3.00E-15
32	1.00E-04	0.15	0.15	0.21	6.32E-02	4.23E-01	0.15	0.21	6.32E-02	4.23E-01	3.00E-15
	1.00E-05	0.15	0.15	0.23	7.72E-02	5.16E-01	0.15	0.23	7.72E-02	5.16E-01	3.00E-15
	1.00E-06	0.15	0.15	0.15	1.66E-04	1.11E-03	0.15	0.15	1.66E-04	1.11E-03	2.00E-15
	1.00E-07	0.15	0.15	0.15	1.80E-06	1.21E-05	0.15	0.15	1.80E-06	1.21E-05	2.00E-15
	1.00E-08	0.15	0.15	0.15	1.33E-08	8.87E-08	0.15	0.15	1.33E-08	8.87E-08	2.00E-15
	1.00E-09	0.15	0.15	0.15	1.58E-08	1.06E-07	0.15	0.15	1.58E-08	1.06E-07	2.00E-15
	1.00E-10	0.15	0.15	0.15	8.62E-11	5.77E-10	0.15	0.15	8.62E-11	5.77E-10	2.00E-15
	1.00E-11	0.15	0.15	0.15	1.43E-11	9.59E-11	0.15	0.15	1.43E-11	9.59E-11	2.00E-15
	1.00E-12	0.15	0.15	0.15	1.18E-12	7.87E-12	0.15	0.15	1.18E-12	7.88E-12	2.00E-15
	1.00E-13	0.15	0.15	0.15	4.32E-13	2.89E-12	0.15	0.15	4.33E-13	2.90E-12	2.00E-15
	1.00E-14	0.15	0.15	0.15	1.80E-14	1.21E-13	0.15	0.15	1.90E-14	1.29E-13	2.00E-15
64	1.00E-04	0.08	0.08	3.62	3.54E+00	4.67E+01	0.08	3.62	3.54E+00	4.67E+01	4.50E-14
	1.00E-05	0.08	0.08	0.09	1.72E-02	2.26E-01	0.08	0.09	1.72E-02	2.26E-01	5.00E-15
	1.00E-06	0.08	0.08	0.08	8.28E-04	1.09E-02	0.08	0.08	8.28E-04	1.09E-02	5.00E-15
	1.00E-07	0.08	0.08	0.08	1.51E-05	2.00E-04	0.08	0.08	1.51E-05	2.00E-04	5.00E-15
	1.00E-08	0.08	0.08	0.08	5.16E-07	6.79E-06	0.08	0.08	5.16E-07	6.79E-06	5.00E-15
	1.00E-09	0.08	0.08	0.08	5.40E-09	7.11E-08	0.08	0.08	5.40E-09	7.11E-08	5.00E-15
	1.00E-10	0.08	0.08	0.08	1.48E-10	1.95E-09	0.08	0.08	1.48E-10	1.95E-09	5.00E-15
	1.00E-11	0.08	0.08	0.08	2.25E-12	2.97E-11	0.08	0.08	2.26E-12	2.97E-11	5.00E-15
	1.00E-12	0.08	0.08	0.08	2.51E-13	3.31E-12	0.08	0.08	2.53E-13	3.34E-12	5.00E-15
	1.00E-13	0.08	0.08	0.08	2.10E-14	2.81E-13	0.08	0.08	2.50E-14	3.26E-13	5.00E-15
	1.00E-14	0.08	0.08	0.08	4.00E-15	5.30E-14	0.08	0.08	7.00E-15	9.40E-14	5.00E-15

Table 5: The initial, minimum and maximum energy values for 1000 time units, in both Euclidean and Fourier space, and the difference between them.

Total Energy in 2 Dimensional Linear ($\beta = 0$) Model

		Physical Space					Fourier Space				
N	Tolerance	Initial	Min	Max	Range (Abs.)	Range (Rel.)	Min	Max	Range (Abs.)	Range (Rel.)	Difference
4x4	1.00E-04	4.77	9.89	4.77	5.11E+00	1.07E+00	9.89	4.77	5.11E+00	1.07E+00	5.00E-15
	1.00E-05	4.77	4.83	4.77	5.84E-02	1.22E-02	4.83	4.77	5.84E-02	1.22E-02	4.00E-15
	1.00E-06	4.77	4.77	4.75	2.26E-02	4.73E-03	4.77	4.75	2.26E-02	4.73E-03	4.00E-15
	1.00E-07	4.77	4.77	4.77	4.23E-05	8.87E-06	4.77	4.77	4.23E-05	8.87E-06	4.00E-15
	1.00E-08	4.77	4.77	4.77	6.91E-05	1.45E-05	4.77	4.77	6.91E-05	1.45E-05	4.00E-15
	1.00E-09	4.77	4.77	4.77	1.76E-04	3.69E-05	4.77	4.77	1.76E-04	3.69E-05	4.00E-15
	1.00E-10	4.77	4.77	4.77	2.46E-05	5.15E-06	4.77	4.77	2.46E-05	5.15E-06	4.00E-15
	1.00E-11	4.77	4.77	4.77	3.40E-06	7.12E-07	4.77	4.77	3.40E-06	7.12E-07	4.00E-15
	1.00E-12	4.77	4.77	4.77	1.85E-08	3.87E-09	4.77	4.77	1.85E-08	3.87E-09	4.00E-15
	1.00E-13	4.77	4.77	4.77	1.95E-09	4.09E-10	4.77	4.77	1.95E-09	4.09E-10	4.00E-15
8x8	1.00E-04	4.88	7.36	4.88	2.48E+00	5.07E-01	7.36	4.88	2.48E+00	5.07E-01	8.00E-15
	1.00E-05	4.88	4.93	4.88	4.66E-02	9.54E-03	4.93	4.88	4.66E-02	9.54E-03	1.00E-14
	1.00E-06	4.88	4.88	4.88	5.88E-04	1.20E-04	4.88	4.88	5.88E-04	1.20E-04	7.00E-15
	1.00E-07	4.88	4.88	4.88	3.53E-04	7.22E-05	4.88	4.88	3.53E-04	7.22E-05	7.00E-15
	1.00E-08	4.88	4.88	4.88	1.10E-06	2.26E-07	4.88	4.88	1.10E-06	2.26E-07	7.00E-15
	1.00E-09	4.88	4.88	4.88	3.71E-07	7.59E-08	4.88	4.88	3.71E-07	7.59E-08	8.00E-15
	1.00E-10	4.88	4.88	4.88	5.92E-09	1.21E-09	4.88	4.88	5.92E-09	1.21E-09	7.00E-15
	1.00E-11	4.88	4.88	4.88	2.38E-09	4.87E-10	4.88	4.88	2.38E-09	4.87E-10	6.00E-15
	1.00E-12	4.88	4.88	4.88	9.06E-09	1.85E-09	4.88	4.88	9.06E-09	1.85E-09	6.00E-15
	1.00E-13	4.88	4.88	4.88	5.33E-09	1.09E-09	4.88	4.88	5.33E-09	1.09E-09	6.00E-15
16x16	1.00E-04	4.92	35.77	4.92	3.08E+01	6.27E+00	35.77	4.92	3.08E+01	6.27E+00	8.50E-14
	1.00E-05	4.92	5.46	4.92	5.35E-01	1.09E-01	5.46	4.92	5.35E-01	1.09E-01	3.60E-14
	1.00E-06	4.92	4.92	4.92	4.06E-05	8.26E-06	4.92	4.92	4.06E-05	8.26E-06	3.60E-14
	1.00E-07	4.92	4.92	4.92	6.28E-05	1.28E-05	4.92	4.92	6.28E-05	1.28E-05	3.50E-14
	1.00E-08	4.92	4.92	4.92	8.34E-06	1.69E-06	4.92	4.92	8.34E-06	1.69E-06	3.30E-14
	1.00E-09	4.92	4.92	4.92	5.77E-08	1.17E-08	4.92	4.92	5.77E-08	1.17E-08	3.20E-14
	1.00E-10	4.92	4.92	4.92	9.50E-09	1.93E-09	4.92	4.92	9.50E-09	1.93E-09	3.60E-14
	1.00E-11	4.92	4.92	4.92	3.31E-09	6.74E-10	4.92	4.92	3.31E-09	6.74E-10	3.20E-14
	1.00E-12	4.92	4.92	4.92	1.53E-09	3.10E-10	4.92	4.92	1.53E-09	3.10E-10	3.30E-14
	1.00E-13	4.92	4.92	4.92	5.94E-11	1.21E-11	4.92	4.92	5.94E-11	1.21E-11	3.40E-14
32x32x	1.00E-04	4.93	12.43	4.92	7.51E+00	1.52E+00	12.43	4.92	7.51E+00	1.52E+00	5.20E-14
	1.00E-05	4.93	8.98	4.93	4.05E+00	8.21E-01	8.98	4.93	4.05E+00	8.21E-01	4.80E-14
	1.00E-06	4.93	4.93	4.93	1.66E-03	3.36E-04	4.93	4.93	1.66E-03	3.36E-04	3.60E-14
	1.00E-07	4.93	4.93	4.93	3.65E-04	7.41E-05	4.93	4.93	3.65E-04	7.41E-05	3.60E-14
	1.00E-08	4.93	4.93	4.93	1.53E-06	3.10E-07	4.93	4.93	1.53E-06	3.10E-07	3.50E-14
	1.00E-09	4.93	4.93	4.93	2.85E-07	5.79E-08	4.93	4.93	2.85E-07	5.79E-08	3.60E-14
	1.00E-10	4.93	4.93	4.93	4.06E-09	8.24E-10	4.93	4.93	4.06E-09	8.24E-10	3.50E-14
	1.00E-11	4.93	4.93	4.93	5.52E-10	1.12E-10	4.93	4.93	5.52E-10	1.12E-10	3.60E-14
	1.00E-12	4.93	4.93	4.93	4.76E-11	9.65E-12	4.93	4.93	4.76E-11	9.65E-12	3.50E-14
	1.00E-13	4.93	4.93	4.93	1.89E-11	3.83E-12	4.93	4.93	1.89E-11	3.83E-12	3.60E-14
64x64	1.00E-04	4.93	4.93	4.93	5.64E-03	1.14E-03	4.93	4.93	5.64E-03	1.14E-03	2.36E-13
	1.00E-05	4.93	5.02	4.93	8.42E-02	1.71E-02	5.02	4.93	8.42E-02	1.71E-02	2.36E-13
	1.00E-06	4.93	4.98	4.93	4.96E-02	1.01E-02	4.98	4.93	4.96E-02	1.01E-02	2.36E-13
	1.00E-07	4.93	4.93	4.93	2.74E-04	5.55E-05	4.93	4.93	2.74E-04	5.55E-05	2.36E-13
	1.00E-08	4.93	4.93	4.93	1.16E-06	2.34E-07	4.93	4.93	1.16E-06	2.34E-07	2.36E-13
	1.00E-09	4.93	4.93	4.93	1.32E-07	2.67E-08	4.93	4.93	1.32E-07	2.67E-08	2.36E-13
	1.00E-10	4.93	4.93	4.93	1.10E-08	2.22E-09	4.93	4.93	1.10E-08	2.22E-09	2.36E-13
	1.00E-11	4.93	4.93	4.93	2.00E-10	4.06E-11	4.93	4.93	2.00E-10	4.06E-11	2.36E-13
	1.00E-12	4.93	4.93	4.93	1.61E-11	3.27E-12	4.93	4.93	1.61E-11	3.26E-12	2.36E-13
	1.00E-13	4.93	4.93	4.93	2.06E-12	4.17E-13	4.93	4.93	2.05E-12	4.16E-13	2.36E-13

Table 6: The initial, minimum and maximum energy values for 1000 time units, in both Euclidean and Fourier space, and the difference between them.

Energy in a straight 8 mass system

Beta	Initial	M(ax)	m(in)	Delta(M-m)	Delta/Init
1	0.283658014	0.283658021	0.283502306	1.56E-04	**5.49E-04**
2	0.295932821	0.295932828	0.295474521	4.58E-04	**1.55E-03**
3	0.308207629	0.308207629	0.307954678	2.53E-04	**8.21E-04**
4	0.320482436	0.320482461	0.320421023	6.14E-05	**1.92E-04**
5	0.332757244	0.332789238	0.332727325	6.19E-05	**1.86E-04**
6	0.345032051	0.345052239	0.345015707	3.65E-05	**1.06E-04**
7	0.357306859	0.35730689	0.357237141	6.97E-05	**1.95E-04**
8	0.369581666	0.369581699	0.369439478	1.42E-04	**3.85E-04**
9	0.381856474	0.381856509	0.38164443	2.12E-04	**5.55E-04**
10	0.394131281	0.394131343	0.393870218	2.61E-04	**6.63E-04**
11	0.406406089	0.406406149	0.406014199	3.92E-04	**9.64E-04**
12	0.418680896	0.41868096	0.4182826	3.98E-04	**9.51E-04**
13	0.430955703	0.430955773	0.43043992	5.16E-04	**1.20E-03**
14	0.443230511	0.443230584	0.442605307	6.25E-04	**1.41E-03**
15	0.455505318	0.45550541	0.454819067	6.86E-04	**1.51E-03**
16	0.467780126	0.467780253	0.46703768	7.43E-04	**1.59E-03**
17	0.480054933	0.480055071	0.479163201	8.92E-04	**1.86E-03**
18	0.492329741	0.492329837	0.491428055	9.02E-04	**1.83E-03**
19	0.504604548	0.504604649	0.503622042	9.83E-04	**1.95E-03**
20	0.516879356	0.516879509	0.515774814	1.10E-03	**2.14E-03**
21	0.529154163	0.529154333	0.528059799	1.09E-03	**2.07E-03**
22	0.541428971	0.541429098	0.540220032	1.21E-03	**2.23E-03**
23	0.553703778	0.553704193	0.552442047	1.26E-03	**2.28E-03**
24	0.565978585	0.565979001	0.56470686	1.27E-03	**2.25E-03**
25	0.578253393	0.5782538	0.57688307	1.37E-03	**2.37E-03**
26	0.5905282	0.590528688	0.589141896	1.39E-03	**2.35E-03**
27	0.602803008	0.60280344	0.601427621	1.38E-03	**2.28E-03**
28	0.615077815	0.615078266	0.61357905	1.50E-03	**2.44E-03**
29	0.627352623	0.627353093	0.625914592	1.44E-03	**2.29E-03**
30	0.63962743	0.639627921	0.638084719	1.54E-03	**2.41E-03**
31	0.651902238	0.651902749	0.650397365	1.51E-03	**2.31E-03**
32	0.664177045	0.664177575	0.662592386	1.59E-03	**2.39E-03**

Table 7: Energy Variation over 4000 time units in a straight 8 mass system.

Energy in straight 32 mass system

Beta	Initial	M(ax)	m(in)	Delta(M-m)	Delta/Init
1	0.074967008	0.074967672	0.074967008	6.64E-07	**0.00E+00**
2	0.075220739	0.075224814	0.075220735	4.08E-06	**1.00E-04**
3	0.075474469	0.075477569	0.0753239	0.00015367	**2.00E-03**
4	0.0757282	0.075729471	0.075659259	7.02E-05	**9.00E-04**
5	0.075981931	0.075982559	0.075819415	0.000163144	**2.10E-03**
6	0.076235661	0.076236185	0.076091725	0.000144459	**1.90E-03**
7	0.076489392	0.076489768	0.076329364	0.000160404	**2.10E-03**
8	0.076743123	0.076743431	0.076499269	0.000244161	**3.20E-03**
9	0.076996853	0.076997189	0.076600413	0.000396776	**5.20E-03**
10	0.077250584	0.077250852	0.076763714	0.000487138	**6.30E-03**
11	0.077504314	0.07750492	0.077097884	0.000407036	**5.30E-03**
12	0.077758045	0.07775829	0.07723701	0.00052128	**6.70E-03**
13	0.078011776	0.078011993	0.077581746	0.000430247	**5.50E-03**
14	0.078265506	0.078265707	0.077945779	0.000319928	**4.10E-03**
15	0.078519237	0.078519463	0.078238158	0.000281305	**3.60E-03**
16	0.078772968	0.07877317	0.078483452	0.000289718	**3.70E-03**
17	0.079026698	0.079026863	0.078724207	0.000302656	**3.80E-03**
18	0.079280429	0.079280609	0.078982839	0.00029777	**3.80E-03**
19	0.079534159	0.07953429	0.079247209	0.000287082	**3.60E-03**
20	0.07978789	0.079788039	0.07951081	0.000277228	**3.50E-03**
21	0.080041621	0.080041784	0.079787171	0.000254613	**3.20E-03**
22	0.080295351	0.080295559	0.080030345	0.000265214	**3.30E-03**
23	0.080549082	0.080549227	0.080317559	0.000231668	**2.90E-03**
24	0.080802813	0.08080294	0.080574834	0.000228105	**2.80E-03**
25	0.081056543	0.081056693	0.08084742	0.000209272	**2.60E-03**
26	0.081310274	0.081310439	0.081099902	0.000210537	**2.60E-03**
27	0.081564005	0.081564123	0.081362797	0.000201327	**2.50E-03**
28	0.081817735	0.081817853	0.081605872	0.000211982	**2.60E-03**
29	0.082071466	0.082071595	0.081854919	0.000216676	**2.60E-03**
30	0.082325196	0.082325338	0.082139632	0.000185706	**2.30E-03**
31	0.082578927	0.082579086	0.082379403	0.000199684	**2.40E-03**
32	0.082832658	0.082832714	0.082639545	0.000193169	**2.30E-03**

Table 8: Energy Variation over 4000 time units in a straight 32 mass system.

Energy in straight 64 mass system

Beta	Initial	M(ax)	m(in)	Delta(M-m)	Delta/Init
1	0.037985868	0.038037933	0.037985868	5.21E-05	**1.37E-03**
2	0.038019108	0.038031302	0.038019108	1.22E-05	**3.21E-04**
3	0.038052348	0.038109016	0.038052348	5.67E-05	**1.49E-03**
4	0.038085588	0.038140194	0.038085588	5.46E-05	**1.43E-03**
5	0.038118828	0.038172772	0.038118828	5.39E-05	**1.42E-03**
6	0.038152068	0.038207933	0.038152068	5.59E-05	**1.46E-03**
7	0.038185308	0.038185471	0.038110284	7.52E-05	**1.97E-03**
8	0.038218548	0.038218592	0.038183902	3.47E-05	**9.08E-04**
9	0.038251788	0.038251816	0.038200963	5.09E-05	**1.33E-03**
10	0.038285028	0.038288409	0.0382432	4.52E-05	**1.18E-03**
11	0.038318268	0.038323256	0.038231295	9.20E-05	**2.40E-03**
12	0.038351508	0.038357968	0.038331519	2.64E-05	**6.90E-04**
13	0.038384749	0.038396304	0.037992682	4.04E-04	**1.05E-02**
14	0.038417989	0.03841811	0.037318567	1.10E-03	**2.86E-02**
15	0.038451229	0.038452743	0.035549459	2.90E-03	**7.55E-02**
16	0.038484469	0.038485868	0.035934045	2.55E-03	**6.63E-02**
17	0.038517709	0.038519085	0.036328461	2.19E-03	**5.69E-02**
18	0.038550949	0.038552198	0.035585422	2.97E-03	**7.70E-02**
19	0.038584189	0.03858538	0.03680849	1.78E-03	**4.61E-02**
20	0.038617429	0.038617442	0.034742277	3.88E-03	**1.00E-01**
21	0.038650669	0.038650683	0.037577801	1.07E-03	**2.78E-02**
22	0.038683909	0.038684843	0.035331111	3.35E-03	**8.67E-02**
23	0.038717149	0.038718379	0.037146701	1.57E-03	**4.06E-02**
24	0.038750389	0.038751435	0.036587783	2.16E-03	**5.58E-02**
25	0.038783629	0.038784856	0.036265622	2.52E-03	**6.50E-02**
26	0.038816869	0.038817836	0.037417632	1.40E-03	**3.61E-02**
27	0.038850109	0.038851489	0.036441297	2.41E-03	**6.20E-02**
28	0.038883349	0.038883973	0.038225358	6.59E-04	**1.69E-02**
29	0.038916589	0.0389177	0.036393303	2.52E-03	**6.49E-02**
30	0.038949829	0.038950843	0.036860207	2.09E-03	**5.37E-02**
31	0.038983069	0.038984202	0.036474403	2.51E-03	**6.44E-02**
32	0.039016309	0.039017397	0.03688209	2.14E-03	**5.47E-02**

Table 9: Energy Variation over 4000 time units in a straight 64 mass system.

Energy in straight 1024 mass system

Beta	Initial	M(ax)	m(in)	Delta(M-m)	Delta/Init
1	0.002407227	0.002660928	0.002407227	2.54E-04	**1.05E-01**
2	0.002407236	0.003356969	0.002407236	9.50E-04	**3.95E-01**
3	0.002407244	0.003350352	0.002407244	9.43E-04	**3.92E-01**
4	0.002407253	0.003316541	0.002407253	9.09E-04	**3.78E-01**
5	0.002407261	0.003551999	0.002407261	1.14E-03	**4.76E-01**
6	0.00240727	0.002939056	0.00240727	5.32E-04	**2.21E-01**
7	0.002407278	0.003337091	0.002407278	9.30E-04	**3.86E-01**
8	0.002407287	0.003543888	0.002407287	1.14E-03	**4.72E-01**
9	0.002407295	0.004005412	0.002407295	1.60E-03	**6.64E-01**
10	0.002407304	0.003339104	0.002407303	9.32E-04	**3.87E-01**
11	0.002407312	0.003265628	0.002407312	8.58E-04	**3.57E-01**
12	0.00240732	0.00240751	0.00240732	1.90E-07	**7.88E-05**
13	0.002407329	0.003509108	0.002407329	1.10E-03	**4.58E-01**
14	0.002407337	0.003585859	0.002407337	1.18E-03	**4.90E-01**
15	0.002407346	0.003733238	0.002407346	1.33E-03	**5.51E-01**
16	0.002407354	0.003269565	0.002407354	8.62E-04	**3.58E-01**
17	0.002407363	0.003454832	0.002407363	1.05E-03	**4.35E-01**
18	0.002407371	0.002407394	0.002407371	2.30E-08	**9.53E-06**
19	0.00240738	0.003611063	0.00240738	1.20E-03	**5.00E-01**
20	0.002407388	0.003277709	0.002407388	8.70E-04	**3.62E-01**
21	0.002407397	0.002881853	0.002407397	4.74E-04	**1.97E-01**
22	0.002407405	0.003430136	0.002407405	1.02E-03	**4.25E-01**
23	0.002407414	0.003217254	0.002407414	8.10E-04	**3.36E-01**
24	0.002407422	0.002407474	0.002407422	5.21E-08	**2.16E-05**
25	0.002407431	0.003823462	0.002407431	1.42E-03	**5.88E-01**
26	0.002407439	0.003220142	0.002407439	8.13E-04	**3.38E-01**
27	0.002407448	0.00336517	0.002407448	9.58E-04	**3.98E-01**
28	0.002407456	0.004288991	0.002407456	1.88E-03	**7.82E-01**
29	0.002407465	0.00408091	0.002407465	1.67E-03	**6.95E-01**
30	0.002407473	0.003220168	0.002407473	8.13E-04	**3.38E-01**
31	0.002407482	0.002407482	0.002407481	6.38E-10	**2.65E-07**
32	0.00240749	0.004240745	0.00240749	1.83E-03	**7.61E-01**

Table 10: Energy Variation over 4000 time units in a straight 1024 mass system.

Energy in square 8×8 mass system

Beta	Initial	M(ax)	m(in)	Delta(M-m)	Delta/Init
1	2.525303809	2.525303816	2.521227865	4.08E-03	**1.61E-03**
2	2.608158759	2.608158765	2.607073013	1.09E-03	**4.16E-04**
3	2.691013709	2.691013723	2.69041248	6.01E-04	**2.23E-04**
4	2.77386866	2.773868682	2.771309842	2.56E-03	**9.22E-04**
5	2.85672361	2.856723953	2.854027448	2.70E-03	**9.44E-04**
6	2.93957856	2.939578986	2.935897246	3.68E-03	**1.25E-03**
7	3.022433511	3.022434115	3.017841407	4.59E-03	**1.52E-03**
8	3.105288461	3.105289066	3.102092711	3.20E-03	**1.03E-03**
9	3.188143411	3.188144032	3.18491073	3.23E-03	**1.01E-03**
10	3.270998362	3.270998995	3.268546753	2.45E-03	**7.50E-04**
11	3.353853312	3.353854071	3.350296371	3.56E-03	**1.06E-03**
12	3.436708262	3.436709041	3.435564843	1.14E-03	**3.33E-04**
13	3.519563213	3.519564011	3.515922743	3.64E-03	**1.03E-03**
14	3.602418163	3.602418981	3.59924127	3.18E-03	**8.82E-04**
15	3.685273113	3.685273952	3.683309234	1.96E-03	**5.33E-04**
16	3.768128064	3.768128915	3.765130608	3.00E-03	**7.96E-04**
17	3.850983014	3.850983883	3.848286125	2.70E-03	**7.01E-04**
18	3.933837964	3.933838847	3.9310002	2.84E-03	**7.22E-04**
19	4.016692915	4.016694133	4.013580286	3.11E-03	**7.75E-04**
20	4.099547865	4.099549144	4.096833769	2.72E-03	**6.62E-04**
21	4.182402815	4.182404135	4.179343092	3.06E-03	**7.32E-04**
22	4.265257766	4.265259124	4.26314011	2.12E-03	**4.97E-04**
23	4.348112716	4.348114092	4.345085167	3.03E-03	**6.97E-04**
24	4.430967666	4.430969132	4.428453482	2.52E-03	**5.68E-04**
25	4.513822617	4.513824164	4.512621867	1.20E-03	**2.66E-04**
26	4.596677567	4.59667914	4.593456132	3.22E-03	**7.01E-04**
27	4.679532517	4.679533997	4.677518745	2.02E-03	**4.31E-04**
28	4.762387468	4.762391188	4.75996757	2.42E-03	**5.09E-04**
29	4.845242418	4.845246237	4.843842729	1.40E-03	**2.90E-04**
30	4.928097368	4.928101401	4.923928272	4.17E-03	**8.47E-04**
31	5.010952319	5.010956451	5.00926568	1.69E-03	**3.37E-04**
32	5.093807269	5.093811304	5.090281826	3.53E-03	**6.93E-04**

Table 11: Energy Variation over 4000 time units in a square 8×8 mass system.

Energy in square 0032×0032 mass system

Beta	Initial	M(ax)	m(in)	Delta(M-m)	Delta/Init
1	2.471817992	2.471818743	2.471814202	4.54E-06	**1.84E-06**
2	2.478097825	2.478142087	2.478088158	5.39E-05	**2.18E-05**
3	2.484377658	2.48437778	2.484360842	1.69E-05	**6.82E-06**
4	2.490657491	2.490657609	2.490634392	2.32E-05	**9.32E-06**
5	2.496937324	2.496998263	2.496936958	6.13E-05	**2.46E-05**
6	2.503217157	2.503217648	2.503158023	5.96E-05	**2.38E-05**
7	2.50949699	2.50950083	2.509388885	1.12E-04	**4.46E-05**
8	2.515776824	2.51837315	2.515776317	2.60E-03	**1.03E-03**
9	2.522056657	2.522066839	2.52191914	1.48E-04	**5.86E-05**
10	2.52833649	2.528585318	2.528335931	2.49E-04	**9.86E-05**
11	2.534616323	2.534638362	2.534337143	3.01E-04	**1.19E-04**
12	2.540896156	2.540898918	2.540496467	4.02E-04	**1.58E-04**
13	2.547175989	2.547435147	2.547170909	2.64E-04	**1.04E-04**
14	2.553455822	2.553763236	2.553364587	3.99E-04	**1.56E-04**
15	2.559735655	2.560224421	2.557102054	3.12E-03	**1.22E-03**
16	2.566015488	2.566018291	2.560094914	5.92E-03	**2.31E-03**
17	2.572295321	2.573463482	2.56603727	7.43E-03	**2.89E-03**
18	2.578575154	2.578683811	2.566634828	1.20E-02	**4.67E-03**
19	2.584854987	2.58489208	2.54965813	3.52E-02	**1.36E-02**
20	2.59113482	2.591171444	2.436809497	1.54E-01	**5.96E-02**
21	2.597414653	2.597455682	2.530486886	6.70E-02	**2.58E-02**
22	2.603694487	2.603701049	2.501675177	1.02E-01	**3.92E-02**
23	2.60997432	2.609998886	2.517800677	9.22E-02	**3.53E-02**
24	2.616254153	2.616274921	2.480729573	1.36E-01	**5.18E-02**
25	2.622533986	2.622541053	2.477476362	1.45E-01	**5.53E-02**
26	2.628813819	2.628813906	2.398628891	2.30E-01	**8.76E-02**
27	2.635093652	2.635093738	2.452334328	1.83E-01	**6.94E-02**
28	2.641373485	2.641373571	2.617173019	2.42E-02	**9.16E-03**
29	2.647653318	2.647653404	2.44986557	1.98E-01	**7.47E-02**
30	2.653933151	2.653933236	2.626419272	2.75E-02	**1.04E-02**
31	2.660212984	2.660213069	2.506262624	1.54E-01	**5.79E-02**
32	2.666492817	2.666492901	2.519782225	1.47E-01	**5.50E-02**

Table 12: Energy Variation over 4000 time units in a square 0032×0032 mass system.

Energy Difference at $t = 0$ ($N = 8$)

Beta	t=9999	t=19999	t=29999	t=39999
1	6.06E-05	9.76E-02	1.05E-02	1.73E+00
2	1.62E+00	9.05E-01	2.02E+00	3.31E+00
3	1.87E+00	1.07E+00	4.17E+00	2.79E+00
4	3.05E+00	3.95E+00	2.06E+00	1.73E+00
5	1.88E+00	2.57E+00	1.57E+00	1.25E+00
6	2.13E+00	2.77E+00	2.07E+00	2.50E+00
7	2.05E+00	2.75E+00	3.11E+00	2.44E+00
8	4.78E+00	1.10E+00	3.17E+00	3.22E+00
9	1.67E+00	3.20E+00	3.60E+00	3.08E+00
10	1.77E+00	1.98E+00	1.91E+00	3.48E+00
11	3.11E+00	3.37E+00	3.36E+00	1.86E+00
12	2.39E+00	1.61E+00	2.76E+00	1.75E+00
13	2.33E+00	3.97E+00	1.62E+00	2.03E+00
14	3.56E+00	2.17E+00	1.76E+00	2.15E+00
15	1.18E+00	2.34E+00	4.94E+00	1.33E+00
16	3.60E+00	2.88E+00	2.48E+00	3.11E+00
17	1.71E+00	1.26E+00	9.57E-01	2.97E+00
18	3.31E+00	2.00E+00	2.55E+00	5.84E+00
19	3.11E+00	1.82E+00	3.08E+00	1.59E+00
20	2.34E+00	2.33E+00	1.67E+00	3.49E+00
21	3.92E+00	4.12E+00	3.40E+00	2.67E+00
22	1.47E+00	3.73E+00	3.23E+00	3.87E+00
23	3.34E+00	3.46E+00	2.90E+00	2.46E+00
24	2.46E+00	2.05E+00	2.83E+00	3.56E+00
25	1.93E+00	2.57E+00	6.17E+00	2.47E+00
26	1.88E+00	1.76E+00	9.10E-01	4.47E+00
27	3.45E+00	2.08E+00	3.42E+00	3.16E+00
28	1.97E+00	4.78E+00	2.69E+00	2.13E+00
29	2.43E+00	3.84E+00	3.84E+00	2.61E+00
30	2.77E+00	4.16E+00	4.32E+00	1.41E+00
31	1.87E+00	2.81E+00	2.71E+00	3.25E+00
32	3.25E+00	1.93E+00	1.55E+00	2.09E+00

Table 13: Energy Difference [(forward's IC minus reverse's LC)/(forward's IC)] after running $N = 8$ mass system forwards t time units, then backwards.

Energy Difference at $t = 0$ ($N = 32$)

Beta	t=9999	t=19999	t=29999	t=39999
1	1.67E-05	8.00E-05	3.48E-04	5.91E-04
2	1.33E-05	1.11E-04	4.68E-04	1.78E-03
3	8.14E-05	5.66E-04	1.54E-03	5.60E-03
4	1.23E-04	1.92E-03	1.22E-03	1.94E-02
5	4.13E-04	8.08E-03	2.01E-02	4.24E-02
6	5.74E-04	6.37E-03	3.77E-02	7.57E-02
7	3.44E-03	1.36E-02	9.19E-03	9.66E-01
8	3.15E-03	3.39E-02	1.77E-01	2.17E+00
9	7.69E-02	3.04E+00	2.25E+00	3.47E+00
10	1.93E-01	1.93E+00	2.87E+00	2.73E+00
11	4.01E-01	2.84E+00	2.38E+00	2.00E+00
12	2.29E+00	2.05E+00	1.90E+00	2.25E+00
13	1.16E+00	1.75E+00	2.38E+00	2.52E+00
14	1.49E+00	2.46E+00	1.40E+00	1.93E+00
15	1.52E+00	1.76E+00	2.01E+00	2.32E+00
16	1.22E+00	2.62E+00	1.54E+00	3.01E+00
17	2.04E+00	3.07E+00	2.58E+00	1.63E+00
18	1.87E+00	2.14E+00	1.76E+00	1.89E+00
19	1.27E+00	2.15E+00	2.06E+00	2.04E+00
20	1.65E+00	2.69E+00	2.40E+00	2.06E+00
21	2.05E+00	1.97E+00	2.11E+00	1.72E+00
22	1.92E+00	2.33E+00	2.32E+00	1.58E+00
23	1.68E+00	2.05E+00	3.12E+00	2.98E+00
24	2.27E+00	2.16E+00	2.03E+00	2.26E+00
25	1.95E+00	1.95E+00	2.47E+00	2.45E+00
26	2.38E+00	2.49E+00	1.95E+00	2.74E+00
27	1.93E+00	2.16E+00	2.66E+00	1.88E+00
28	2.44E+00	2.71E+00	2.48E+00	2.15E+00
29	2.44E+00	2.23E+00	2.18E+00	2.54E+00
30	2.38E+00	1.83E+00	2.67E+00	2.64E+00
31	2.68E+00	2.55E+00	1.69E+00	1.55E+00
32	1.87E+00	2.52E+00	2.68E+00	2.04E+00

Table 14: Energy Difference [(forward's IC minus reverse's LC)/(forward's IC)] after running $N = 32$ mass system forwards t time units, then backwards.

Energy Difference at $t = 0$ ($N = 64$)

Beta	t=9999	t=19999	t=29999	t=39999
1	1.67E-05	8.00E-05	3.48E-04	5.91E-04
2	1.33E-05	1.11E-04	4.68E-04	1.78E-03
3	8.14E-05	5.66E-04	1.54E-03	5.60E-03
4	1.23E-04	1.92E-03	1.22E-03	1.94E-02
5	4.13E-04	8.08E-03	2.01E-02	4.24E-02
6	5.74E-04	6.37E-03	3.77E-02	7.57E-02
7	3.44E-03	1.36E-02	9.19E-03	9.66E-01
8	3.15E-03	3.39E-02	1.77E-01	2.17E+00
9	7.69E-02	3.04E+00	2.25E+00	3.47E+00
10	1.93E-01	1.93E+00	2.87E+00	2.73E+00
11	4.01E-01	2.84E+00	2.38E+00	2.00E+00
12	2.29E+00	2.05E+00	1.90E+00	2.25E+00
13	1.16E+00	1.75E+00	2.38E+00	2.52E+00
14	1.49E+00	2.46E+00	1.40E+00	1.93E+00
15	1.52E+00	1.76E+00	2.01E+00	2.32E+00
16	1.22E+00	2.62E+00	1.54E+00	3.01E+00
17	2.04E+00	3.07E+00	2.58E+00	1.63E+00
18	1.87E+00	2.14E+00	1.76E+00	1.89E+00
19	1.27E+00	2.15E+00	2.06E+00	2.04E+00
20	1.65E+00	2.69E+00	2.40E+00	2.06E+00
21	2.05E+00	1.97E+00	2.11E+00	1.72E+00
22	1.92E+00	2.33E+00	2.32E+00	1.58E+00
23	1.68E+00	2.05E+00	3.12E+00	2.98E+00
24	2.27E+00	2.16E+00	2.03E+00	2.26E+00
25	1.95E+00	1.95E+00	2.47E+00	2.45E+00
26	2.38E+00	2.49E+00	1.95E+00	2.74E+00
27	1.93E+00	2.16E+00	2.66E+00	1.88E+00
28	2.44E+00	2.71E+00	2.48E+00	2.15E+00
29	2.44E+00	2.23E+00	2.18E+00	2.54E+00
30	2.38E+00	1.83E+00	2.67E+00	2.64E+00
31	2.68E+00	2.55E+00	1.69E+00	1.55E+00
32	1.87E+00	2.52E+00	2.68E+00	2.04E+00

Table 15: Energy Difference [(forward's IC minus reverse's LC)/(forward's IC)] after running $N = 64$ mass system forwards t time units, then backwards.

Energy Difference at $t = 0$ ($N = 1024$)

Beta	t=9999	t=19999	t=29999	t=39999
1	5.59E-08	1.64E-07	3.49E-07	5.24E-07
2	5.79E-08	1.60E-07	3.17E-07	4.70E-07
3	5.02E-08	1.54E-07	2.91E-07	4.65E-07
4	5.37E-08	1.62E-07	3.01E-07	4.75E-07
5	5.09E-08	1.66E-07	2.95E-07	4.90E-07
6	5.43E-08	1.40E-07	2.46E-07	4.45E-07
7	6.00E-08	1.40E-07	2.75E-07	5.46E-07
8	5.58E-08	1.39E-07	2.72E-07	5.38E-07
9	4.97E-08	1.58E-07	2.86E-07	4.75E-07
10	6.01E-08	1.78E-07	2.84E-07	5.72E-07
11	5.19E-08	1.52E-07	3.00E-07	5.07E-07
12	4.81E-08	1.36E-07	2.60E-07	4.81E-07
13	5.07E-08	1.54E-07	3.01E-07	5.31E-07
14	6.03E-08	1.74E-07	3.05E-07	5.31E-07
15	5.50E-08	1.41E-07	2.62E-07	4.29E-07
16	5.34E-08	1.38E-07	2.58E-07	4.87E-07
17	5.50E-08	1.63E-07	3.07E-07	5.01E-07
18	7.23E-08	1.67E-07	2.95E-07	5.19E-07
19	5.66E-08	1.59E-07	2.77E-07	4.84E-07
20	5.16E-08	1.39E-07	2.71E-07	4.58E-07
21	5.62E-08	1.29E-07	2.52E-07	4.37E-07
22	5.55E-08	1.45E-07	2.83E-07	4.88E-07
23	5.81E-08	1.58E-07	2.99E-07	4.31E-07
24	5.01E-08	1.30E-07	2.64E-07	4.39E-07
25	5.34E-08	1.42E-07	2.66E-07	4.62E-07
26	6.19E-08	1.44E-07	2.94E-07	4.87E-07
27	5.71E-08	1.41E-07	2.96E-07	4.74E-07
28	5.31E-08	1.43E-07	2.64E-07	4.63E-07
29	5.98E-08	1.49E-07	2.99E-07	4.95E-07
30	5.38E-08	1.46E-07	2.68E-07	4.79E-07
31	6.09E-08	1.39E-07	2.48E-07	4.71E-07
32	5.57E-08	1.49E-07	2.79E-07	4.59E-07

Table 16: Energy Difference [(forward's IC minus reverse's LC)/(forward's IC)] after running $N = 1024$ mass system forwards t time units, then backwards.

Energy Difference at $t = 0$ ($N = 8 \times 8$)

Beta	t=9999	t=19999	t=29999	t=39999
1	1.07E-01	1.75E+00	8.14E+00	1.83E+01
2	1.92E-01	3.49E+00	1.93E+01	3.94E+01
3	1.42E-01	5.16E+00	2.64E+01	4.36E+01
4	5.61E-01	9.12E+00	4.94E+01	1.83E+00
5	7.57E-01	8.80E+00	3.12E+01	5.52E+00
6	3.05E-01	9.78E+00	5.78E+01	4.03E+00
7	7.72E-01	1.97E+01	5.75E+01	8.51E-02
8	3.18E+01	2.32E+01	2.51E+01	1.58E+01
9	1.94E+01	1.89E+01	1.96E+01	2.00E+01
10	7.39E-01	9.81E+00	5.22E+01	5.04E+01
11	6.09E-01	6.82E+00	8.21E+01	6.42E-02
12	4.24E-01	2.46E+01	3.54E+01	6.47E+00
13	7.17E-01	6.36E+00	7.78E+01	7.26E+01
14	1.53E+01	2.71E+01	2.75E+01	2.54E+01
15	1.87E+01	2.16E+01	2.21E+01	2.42E+01
16	3.00E+01	2.73E+01	2.13E+01	2.39E+01
17	1.24E+00	2.54E+01	2.60E+01	1.86E+01
18	3.03E-01	2.22E+01	1.40E+01	2.39E+01
19	2.81E+01	2.34E+01	2.68E+01	2.59E+01
20	2.42E+01	2.78E+01	2.14E+01	3.41E+01
21	2.72E+01	2.80E+01	3.13E+01	1.90E+01
22	2.79E+01	1.66E+01	2.16E+01	3.06E+01
23	2.77E+01	2.59E+01	1.78E+01	2.40E+01
24	3.14E+01	2.48E+01	2.38E+01	2.70E+01
25	2.36E+01	3.88E+01	3.28E+01	3.14E+01
26	3.20E+01	3.21E+01	2.92E+01	1.97E+01
27	2.99E+01	2.48E+01	2.80E+01	2.44E+01
28	3.63E+01	3.49E+01	3.49E+01	3.49E+01
29	2.34E+01	2.38E+01	3.65E+01	3.65E+01
30	3.13E+01	3.46E+01	3.15E+01	2.59E+01
31	3.09E+01	3.09E+01	3.09E+01	3.09E+01
32	3.16E+01	2.82E+01	2.82E+01	2.82E+01

Table 17: Energy Difference [(forward's IC minus reverse's LC)/(forward's IC)] after running $N = 8 \times 8$ mass system forwards t time units, then backwards.

Energy Difference at $t = 0$ ($N = 32 \times 32$)

Beta	t=9999	t=19999	t=29999	t=39999
1	1.04E-04	1.14E-03	4.17E-03	9.63E-03
2	1.39E-04	9.56E-04	2.75E-03	2.34E-02
3	1.05E-04	1.13E-03	5.30E-03	3.62E-02
4	1.08E-04	8.91E-04	7.27E-03	5.40E-02
5	1.22E-04	1.05E-03	1.01E-02	8.42E-02
6	1.13E-04	1.35E-03	1.24E-02	1.06E-01
7	1.24E-04	1.80E-03	1.87E-02	1.63E-01
8	1.41E-04	1.68E-03	2.30E-02	1.99E-01
9	1.51E-04	1.89E-03	2.34E-02	2.17E-01
10	1.67E-04	2.01E-03	2.83E-02	2.54E-01
11	1.88E-04	2.20E-03	3.13E-02	2.64E-01
12	2.16E-04	2.94E-03	4.10E-02	3.73E-01
13	2.76E-04	3.36E-03	4.39E-02	3.96E-01
14	3.61E-04	4.22E-03	4.78E-02	4.24E-01
15	8.20E-04	2.51E-02	2.92E-01	1.78E+00
16	7.07E-04	8.21E-03	5.50E-02	4.00E-01
17	1.24E-03	2.13E-02	1.11E-01	4.76E-01
18	1.10E-03	1.61E-02	1.64E-01	1.05E+00
19	1.93E-03	4.89E-02	6.42E-01	7.83E+00
20	5.23E-03	3.94E+00	4.77E+00	5.01E+00
21	1.10E-02	2.06E-01	5.07E+00	8.99E+00
22	7.69E-02	6.98E+00	9.42E+00	7.64E+00
23	1.16E+01	1.09E+01	1.45E+01	1.55E+01
24	1.15E+01	1.01E+01	8.15E+00	7.68E+00
25	1.25E+01	7.52E+00	3.94E+00	7.02E+00
26	1.64E+01	6.27E+00	6.98E+00	9.33E+00
27	1.24E+01	1.18E+01	7.13E+00	8.27E+00
28	1.01E+01	9.45E+00	1.15E+01	1.69E+01
29	4.96E+00	1.03E+01	7.46E+00	6.81E+00
30	8.30E+00	6.25E+00	1.17E+01	1.05E+01
31	9.62E+00	5.90E+00	4.71E+00	5.95E+00
32	1.04E+01	4.22E+00	1.09E+01	1.08E+01

Table 18: Energy Difference [(forward's IC minus reverse's LC)/(forward's IC)] after running $N = 32 \times 32$ mass system forwards t time units, then backwards.